TORION

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User's Manual

TRIDION™-9

Gas Chromatograph-Toroidal Ion Trap
Mass Spectrometer (GC-TMS)

TORION® TECHNOLOGIES INC.

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Version 2.0.1
May 2012

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Chapter 1

1 Introduction

This chapter contains a brief introduction to the TRIDION® and CUSTODION® products.

This user's manual provides step-by-step instructions for operating and trouble-shooting the TRIDION GC-TMS and the CUSTODION line of solid phase microextraction (SPME) syringes. Both basic operations (such as running a sample and changing the batteries) and advanced operations (such as re-analyzing data and changing the instrument operating parameters) are included.

The TRIDION is used to separate and identify volatile and semi-volatile organic compounds present in gas, liquid and solid samples. The CUSTODION SPME syringe is used to extract various classes of compounds (depending on the sorbent coating of the fiber) and to concentrate the sample for improved sensitivity at low concentrations. The CUSTODION is used to introduce the sample into the TRIDION.

After injecting a sample into the TRIDION it is separated into its chemical components. Resolved components are characterized by retention time from the gas chromatograph (GC) and mass spectral fingerprint from the toroidal ion trap mass spectrometer (TMS). The mass spectral fingerprints of the chemicals are compared to a database of known mass spectral fragmentation patterns, and are identified by the on-board library.

Chapter 2

2 Tutorial

This chapter provides a tutorial about solid phase microextraction (SPME), low thermal mass (LTM) gas chromatography (GC) and toroidal ion trap mass spectrometry (TMS).

What is solid phase microextraction (SPME)?

Solid phase microextraction (SPME) is a sampling method for extracting target chemicals from a gas, liquid or dissolved solid sample and concentrating them for subsequent analysis. Compared to liquid-liquid extraction and cartridge-based solid phase extraction, SPME is faster and less prone to user error. Following extraction, SPME allows immediate introduction of sample into the analytical instrument.

SPME consists primarily of a fused silica or metal rod that is approximately one centimeter in length and a tenth of a millimeter in diameter. The rod is typically coated with a polymeric material called a sorbent. The rod and sorbent together are referred to as the SPME fiber. The chemical properties of the sorbent determine the classes of compounds that selectively absorb or adsorb onto the fiber. Solvents should not absorb preferentially over target chemicals, otherwise a different sorbent or solvent may be necessary.

1. The SPME fiber is stored inside a protective needle called the SPME needle. The fiber is extended out of the SPME needle during the extraction and desorption of a sample. The SPME needle is connected to a spring loaded plunger that extends and retracts the fiber. The complete apparatus is called the SPME syringe.

2. Each chemical is extracted into the SPME coating according to its equilibrium distribution between the coating on the fiber and the liquid (or gas) phase around the fiber. This equilibrium depends on the chemical nature of the polymeric phase, the solvent, the temperature, and the volume of both the polymeric phase and the solvent. Extraction can take under a minute depending on sample volume and concentration. Equilibration of the fiber with its surrounding matrix usually requires a longer period of time (several minutes to several hours). After equilibrium has been achieved, the concentrations of target chemicals on the fiber and in the solution remain constant. The amount of a chemical extracted by the fiber is proportional to the concentration of the sample before and after equilibrium.

3. Sensitivity to a target chemical extracted by SPME can be improved significantly in three ways: increasing the sorbent thickness on the sampling fiber, employing a more selective sorbent, or changing the extraction temperature. A thicker sorbent layer absorbs more target chemical, increasing the sensitivity to all absorbed chemicals; however, thicker sorbent also increases the equilibration time between the absorbed chemical and the chemical in solution. Rather than thicker sorbent, longer fibers may be used to increase sensitivity; however, longer fibers may not be used on the TRIDION, the instrument is not designed to accept them and they may break inside the injection port. Sorbents with greater selectivity to the target chemicals will improve sensitivity; however, they may also increase the extraction of unwanted chemicals. Finally, changing the extraction temperature will affect the sensitivity of a target chemical. The sensitivity for high mass and high boiling chemicals will generally improve with increased temperature, particularly for headspace (gas) extractions. Increasing the temperature will also decrease the equilibration time. High temperature

extractions of volatile chemicals in solution may decrease the sensitivity to those chemicals when sampling by immersion because volatile chemicals are more likely to leave the solution as vapor at higher temperatures.

What is the CUSTODION SPME syringe?

1. The SPME syringe designed for the TRIDION is called the CUSTODION. The CUSTODION triggers the injection and analysis to start on the TRIDION without having to push a "start analysis" button.

2. The SPME syringe consists primarily of a barrel, plunger, spring, protective needle, and fiber.

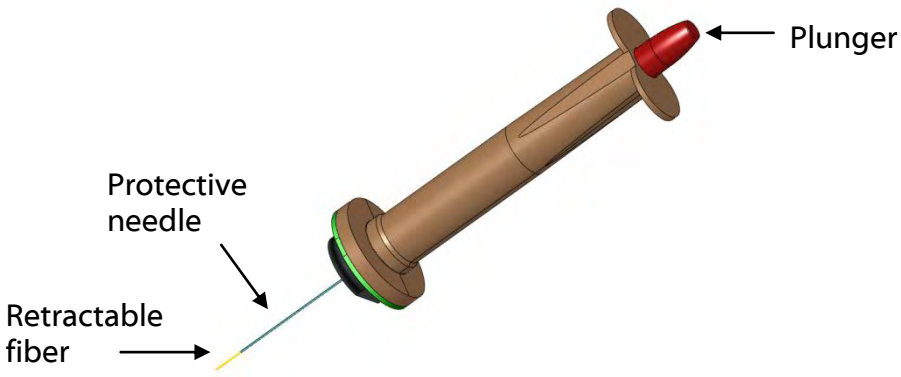


Figure 2-1Diagram of the CUSTODION sampling syringe

What is low thermal mass (LTM) gas chromatography (GC)?

1. In microcolumn gas chromatography (GC), volatile chemicals separate as they travel through a capillary column. Separation is dependent upon the equilibrium distribution of each chemical between a liquid coating on the capillary wall and the carrier gas flowing through the capillary. An equilibrium constant called the partition coefficient, K, governs the separation of chemicals and is a ratio of the concentration of the target chemical in the stationary phase coating versus the mobile phase (carrier gas). The affinity of a chemical for the stationary phase is a function of temperature and determines the chemical's partitioning between the two phases.

$$K = \frac{concentrat\,ion\ in\ stationary\ \ phase}{concentrat\,ion\ in\ mobile\ \ phase} = \frac{mass\ in\ stationary\ \ phase}{mass\ in\ mobile\ \ phase} \times \frac{volume\ in\ mobile\ \ phase}{volume\ in\ stationary\ \ phase}$$

2. The partition coefficient of a chemical is related to its retention time, t_R. The retention time is the time a chemical takes to travel through the column. The typical representation of a GC analysis is a plot of detector response as a function of time, called a chromatogram (see figure 2.2). The time at the center of the near Gaussian peak of a resolved chemical is its retention time, and the area under the peak is related to the amount of chemical extracted and may be corresponded to the amount of chemical in the sample.

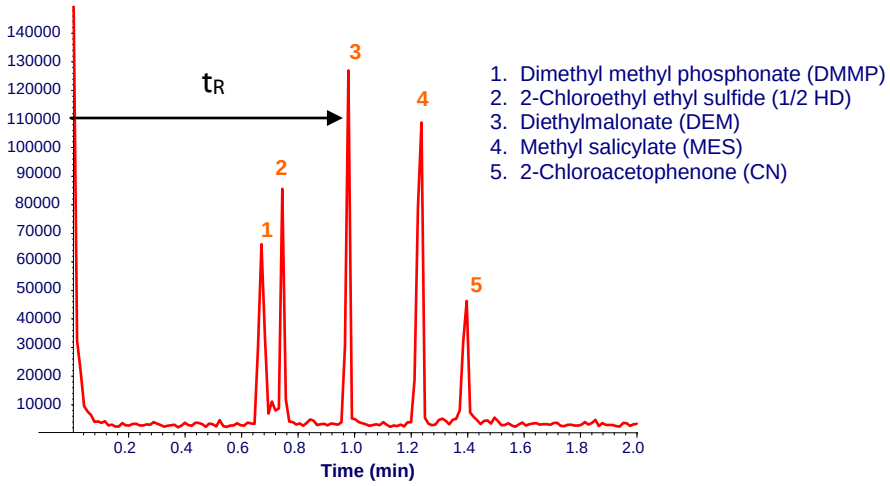


Figure 2-2 Typical chromatogram obtained using the TRIDION GC-TMS showing the retention time of diethylmalonate

3. A chemical that is volatile within the temperature range of the GC method parameters will eventually exit the column (assuming the compound is not irreversibly adsorbed to the capillary coating). If the same method parameters are always used, a specific chemical will have the same retention time. Tentative identification of a chemical can be made by comparing its retention time with retention times of known standards. Changing the temperature of the capillary column will change the retention times of compounds being analyzed. Usually, the temperature of the column is increased during an analysis to reduce the time of the analysis. This is typically done with the capillary column installed in a convectively heated GC oven.

4. The degree of separation of two chemicals that exit the capillary column at the detector is called resolution. Two chromatographic peaks are completely resolved when the baseline signal is present between them; otherwise, they are only partially resolved. Adequate resolution between peaks is necessary to allow the use of retention times for tentative chemical identification and to produce sufficiently accurate mass spectral fingerprints for positive identification. Peaks with similar retention times may be resolved by reducing their peak widths or by changing their relative retention times.

5. Low thermal mass (LTM) GC refers to a miniaturized form of GC in which the convectively heated column oven is replaced with direct electrical resistive heating of the capillary column. LTM GC uses a conventional GC column that is intertwined with resistive heating and temperature-sensing wires and wrapped with aluminum foil for greater heating efficiency. The low thermal mass of this column heating arrangement allows for much smaller instrumentation and lower operating power as well as faster heating and cooling of the column. The GC in the TRIDION is an LTM GC.

What is toroidal ion trap mass spectrometry (TMS)?

1. The purpose of mass spectrometry (MS) is to measure the presence and abundance of a chemical's characteristic ion fragments according to the values of their mass-to-charge ratios (*m/z*). MS involves several steps to generate a mass spectrum of a chemical: ionization, mass analysis, and detection.

2. Ionization is necessary for producing electrically charged fragments (i.e., ions). A plot of the abundances of ions produced from a chemical as a function of *m/z* is called a mass spectrum. Each chemical has a characteristic mass spectrum that can be used as a chemical fingerprint to identify the chemical and differentiate it from other chemicals. Soft ionization methods primarily produce

molecular ions or ions related to the molecular ion (e.g., abstraction of hydrogen or addition of hydrogen or other species). Hard ionization processes yield fragments of the chemicals.

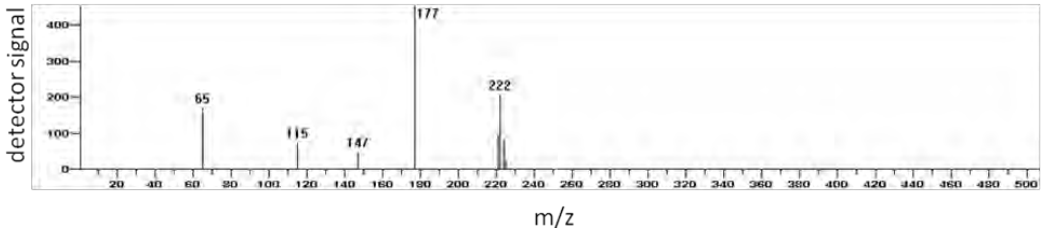


Figure 2-3 Mass spectrum obtained by the TRIDION showing the mass-to-charge (m/z) of ionized fragments of diethyl phthalate

3. Electron ionization is a hard ionization method in which the sample intersects an energetic (e.g., 70 eV) beam of electrons that are drawn from a current-carrying filament. The interaction of the chemicals in the sample and the electrons in the electron beam creates charged fragments.

4. The ionized chemical fragments are separated by a mass analyzer before they are registered by the detector. Typical mass analyzers include quadrupole, time-of-flight, and ion traps. The TRIDION uses a miniaturized toroidal ion trap (TMS) mass analyzer that possesses advantages of simplicity, low power consumption, and high sensitivity. Mass analysis is accomplished by first trapping ions in the trap with an RF and then applying a constant frequency tickle voltage as the RF voltage is increased, causing ions to be ejected from the ion trap to the detector based on *m/z* and their resonant frequency for ejection. Discrete ranges (windows) of the *ejection RF voltage* are assigned to discrete *m/z* values of the detected ions.

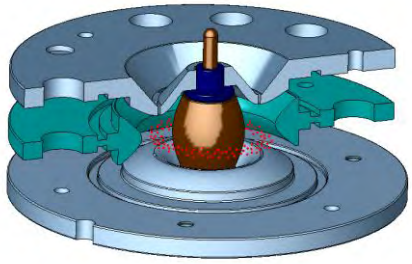


Figure 2-4 Cut-away drawing of the toroidal ion trap showing trapping of ions (red dots) in a toroidal geometry around the center electrode

5. Ion detection provides the abundances of the fragment ions in the mass spectrum. The detector in the TRIDION is a continuous dynode electron multiplier. Positive ions exiting the trap are directed by a negative bias to strike a surface at the entrance of the detector. The surface emits electrons when struck by ions with sufficient energy. The electrons are directed by a positive bias striking further along the continuous dynode, emitting increasingly more electrons as they sequentially strike the dynode in areas of decreasing negative voltage. The positive bias ultimately directs the electrons to a collector at the end of the continuous dynode, that produces a measurable voltage that is proportional to the number of ions of each type (i.e., *m/z* value) isolated by the mass analyzer.

6. A variety of mass analyzers are available for laboratories, however, few are available as portable instruments due to overall size and power requirements. The latest advancement in miniaturization of mass spectrometers is the miniaturized TMS (see figure 2.4 and 2.5). The miniaturized TMS requires less power, and operates under higher pressures than quadrupole mass spectrometers. Furthermore, the miniaturized TMS combines many advantages of larger non-toroidal ion traps, such as simplicity, pressure tolerance, and comparable ion storage volume. The miniature TMS operates at less than 2.5 kV, compared to 15 kV for the larger alternative portable ion trap.

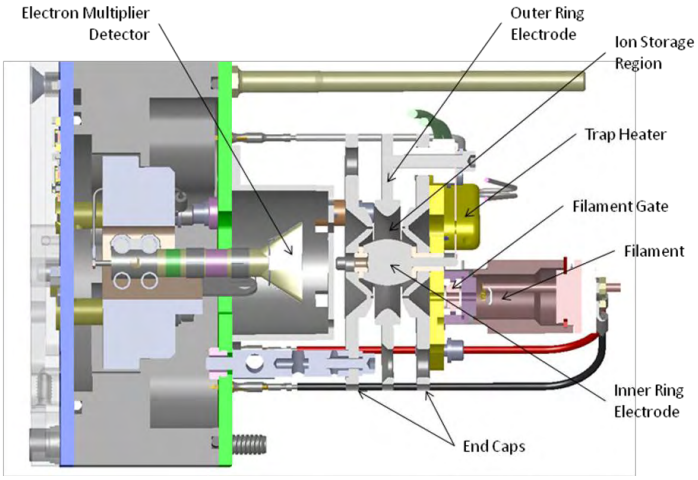


Figure 2-5 Diagram of the TMS assembly with ion source (filament) and electron multiplier detector

What is the TRIDION?

1. The TRIDION (Figure 2.6) is an easy to use, hand-portable GC-TMS system. The primary purpose of the TRIDION is to allow rapid chemical analysis and detection on-site so that informed decisions based on chemical analysis can be made as quickly as possible. The combination of low thermal mass GC and TMS allows rapid separation of chemicals in the sample and generation of a mass spectral fingerprint for each chemical. The on-board central processing unit (CPU) compares the retention time and mass spectrum of each chemical to a library of retention times and mass spectra of known chemicals, and indicates whether or not any of the target chemicals in the library are present in the sample.

2. The front panel of the TRIDION contains the battery compartment, display screen, power and operating buttons, SPME sample injection port, memory card slot, Ethernet port, carrier gas cartridge connection, status lights, and manual shut-off access. The internal components are precision mechanical and electronic parts, including heaters, vacuum pumps, pressure controller, gas flow lines, circuit boards, CPU, SPME injector, low thermal mass GC, and TMS.

Figure 2-6 TRIDION GC-TMS

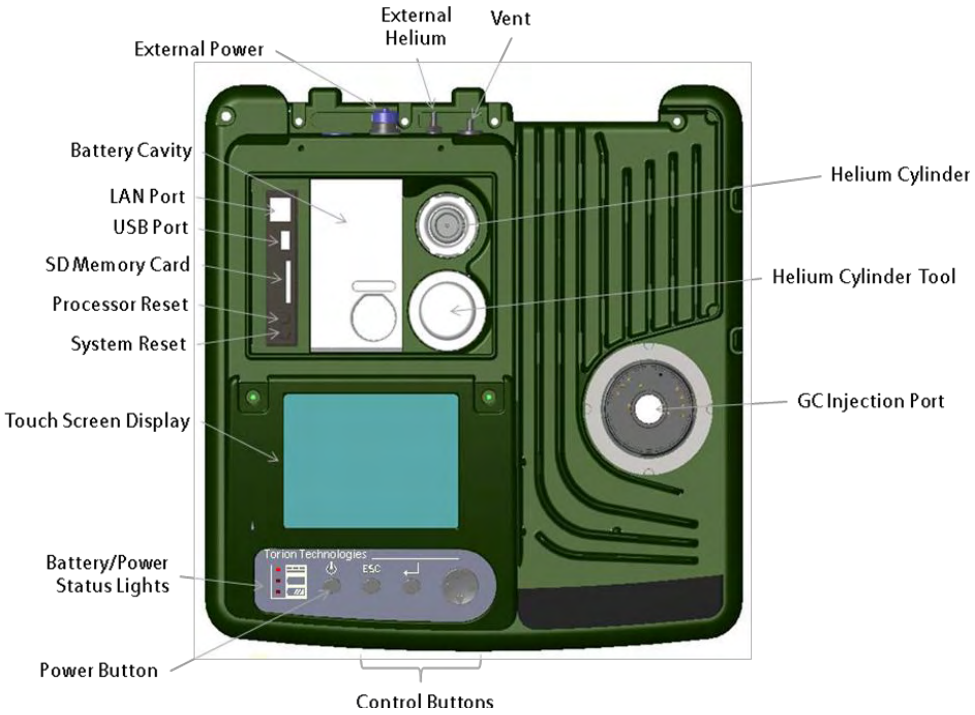


Figure 2-7 Top view TRIDION GC-TMS

Chapter 3

3 Basic CUSTODION Operations

This chapter gives basic instructions on how to use the CUSTODION.

Prepare the CUSTODION SPME syringe for sampling

Each CUSTODION SPME syringe is shipped with the syringe needle protected by a screw-tight cap. Prior to use, remove the protective cap. Prior to initial use, the SPME fiber should be conditioned by placing it in a heated GC injection port for at least 15 minutes. For multiple-use application, the SPME fiber in the CUSTODION syringe should be cleaned before re-use as outlined in the following steps:

1 Insert the syringe needle (with the fiber retracted) of the CUSTODION syringe into the injection port of the TRIDION or other GC (heated to at least 250°C).

2 Depress the plunger to extend the SPME fiber and allow the fiber to desorb contaminants for 30–60 seconds or longer if necessary.

3 Depress the plunger to retract the SPME fiber.

4 Remove the CUSTODION syringe needle from the injection port.

5 Start the TRIDION and conduct a System Blank Run to remove any compounds that may have desorbed from the SPME fiber into the GC (for instructions on performing a System Blank Run see the TRIDION Operation chapter).

6 If large amounts of sample are visible in the blank analysis repeat the SPME cleaning process until no large peaks are visible in the System Blank Run.

Using the CUSTODION

1. Detection of target chemicals by the TRIDION depends on adsorption to (extraction) and desorption from (injection) the SPME fiber. Adsorption depends on the partition coefficient of the target chemical between the fiber coating and the sample matrix. Detection also depends on the volatility and molecular mass of the target chemical (45–500 amu).

Sample headspace vapors from liquid or solid samples

Place the liquid or solid sample into a vial. Leave sufficient volume (headspace) above the sample for sampling vapors when the SPME fiber is fully extended from the CUSTODION syringe needle.

1. Cap the vial with a septum cap.

2. Insert the CUSTODION needle through the sample vial septum.

Caution!

Be certain that the SPME fiber is retracted inside the CUSTODION needle (i.e., protective needle) before piercing it through the sample vial septum.

Caution!

Be careful not to bend the flexible SPME needle when piercing the septum.

Caution!

Try to keep the CUSTODION syringe needle above the surface of the sample to prevent uptake of liquid onto the SPME fiber by capillary action.

3. Depress the CUSTODION plunger to extend the fiber into the headspace sample.

Note

Depress the plunger until you hear or feel a click and then release the plunger.

4. After the desired extraction time, depress the plunger to retract the fiber into the syringe needle.

5. Remove the CUSTODION syringe needle from the sample vial.

Caution!

Be certain that the SPME fiber is completely retracted before pulling the CUSTODION syringe needle out through the sample septum.

Sample gases

1. Vapors in air or other gas samples can be sampled directly or from a gas sampling container using the CUSTODION syringe. The steps for vapor headspace analysis (as discussed above) should be followed when applicable.

Sample liquids

Caution!

Samples that are too concentrated will overload the GC column and TMS, possibly requiring cleaning of the system (CUSTODION SPME fiber, ion trap, etc.) before the next sample can be analyzed. Of particular concern is the viscosity of the liquid sample. Viscous samples should never be sampled and analyzed directly.

1. Place the liquid or dissolved solid sample into a sample vial. Add sufficient volume of liquid to completely immerse the SPME fiber when it is fully extended from the CUSTODION syringe needle.

2. Cap the vial with a septum cap.

3. Insert the CUSTODION syringe needle through the sample vial septum.

Caution!
Be certain that the SPME fiber is retracted inside the CUSTODION syringe needle before piercing it through the sample vial septum.

Caution!
Be careful not to bend the flexible SPME needle when piercing the septum.

4. Check for adequate space inside the vial to extend the CUSTODION fiber without touching the sides or bottom of the vial.

5. Depress the CUSTODION plunger to extend the fiber into the sample and start the timer. Carefully swirl (agitate) the liquid sample in the vial around the SPME fiber to increase contact of the fiber coating with as much of the total sample volume as possible, making certain that the fiber coating is always covered with the liquid sample.

Caution!
Make certain that there is enough liquid in the sample vial to completely cover the SPME fiber coating when it is extended into the sample and the sample is agitated.

6. After the desired extraction time, depress the CUSTODION plunger to retract the fiber into the syringe needle.

7. Remove the CUSTODION syringe needle from the sample vial.

Caution!
Be certain that the SPME fiber is completely retracted before pulling the CUSTODION syringe needle out through the sample septum.

8. Prior to injection on the TRIDION, extend the SPME fiber out of the CUSTODION syringe needle and shake off residual sample droplets that may have been taken up in the syringe needle during sampling.

Sample solids

1. Always perform vapor headspace analysis of a solid sample as described above before attempting other sampling methods.

2. Dissolve (or suspend) a small amount of the solid sample in the appropriate solvent and follow steps **2**–**8** as described above for sampling liquids.

Sample unknown liquids and solids

1. The following two pages provide sequential procedures for trouble-shooting liquid and solid unknowns that are too dilute or too concentrated when initially sampled by headspace. The first

step with any unknown compound is to sample the headspace. If detection of target chemicals is too low or too high, follow the flow chart on the next two pages to improve detection.

2. Each box in the flow chart provides a new method for sample preparation to increase or decrease the concentration of extracted chemicals. If the results are not improved by performing the method in the first box, move on to the next box and perform the subsequent sample handling procedure.

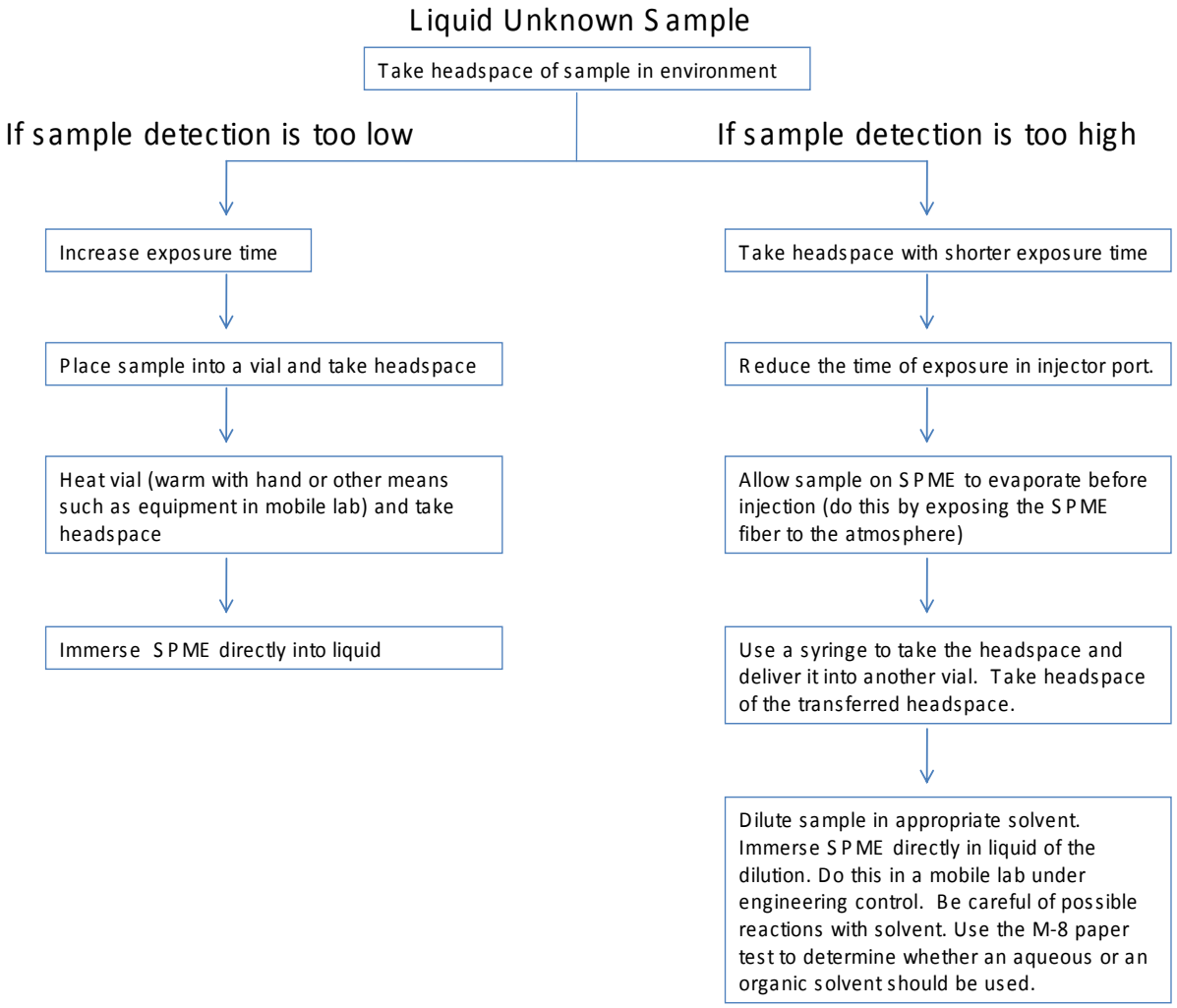


Table 3-1 Liquid unknown sample flow chart

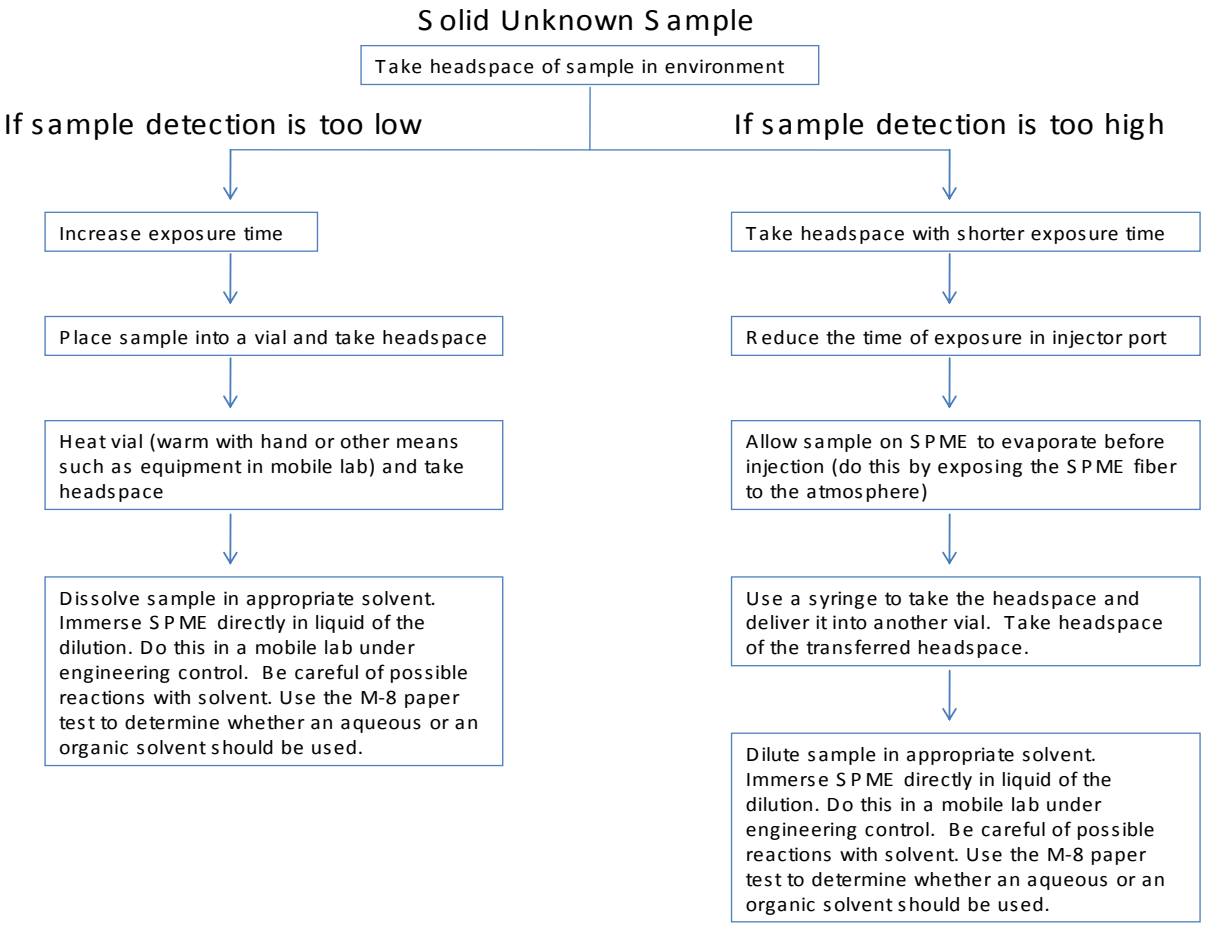


Table 3-2 Solid unknown sample flow chart

Performing an Injection with the CUSTODION Syringe

1. When performing an injection with the CUSTODION Syringe on the TRIDION-9 make sure the gold rings on the CUSTODION Syringe touch the contact points on the GC injection port. When the contact points connect with the CUSTODION Syringe the instrument automatically starts a run.

2. Conversely the instrument will NOT start an analysis if the CUSTODION Syringe does not come in contact with the contact points.

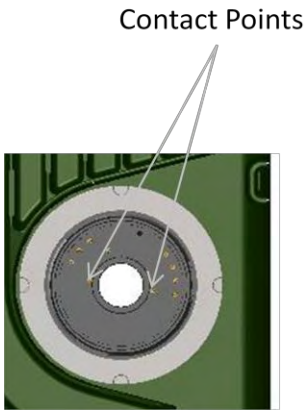


Figure 3-1 Interface between the SPME syringe and the injector

3. Follow the on screen instructions as to when to depress the plunger to expose the SPME fiber.

4. Depress the plunger until you hear or feel a click and then release the plunger. Similar to a ball point pen.

5. The following image shows a cutaway diagram of the SPME inside the GC injector port.

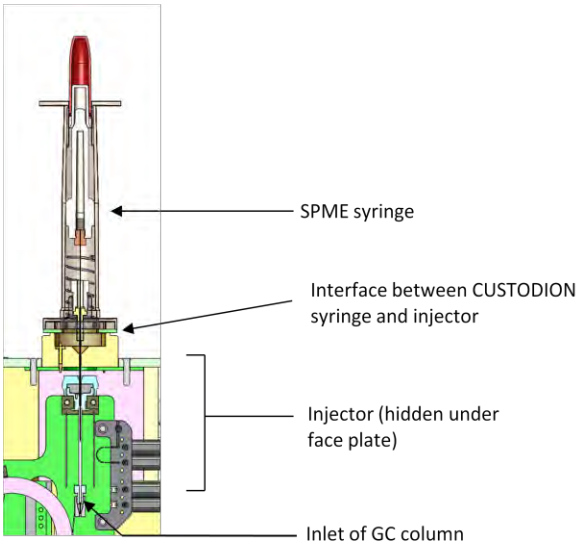


Figure 3-2 Cutaway diagram of CUSTODION syringe inserted into the injector port with fiber retracted

6. Follow the on screen instructions as to when to depress the plunger to retract the SPME fiber inside the protective needle.

Caution!

Ensure the SPME fiber is completely withdrawn inside the syringe needle before removing the CUSTODION from the injector port, otherwise SPME fiber may be damaged.

Chapter 4

4 Instrument Operation

This chapter describes the functionality of the instrument control interface. This includes a description of each screen and the functions available from the screen.

Basic Functions

1. The user interface is run using Windows CE™ as the operating system.

2. Upon initialization the software will automatically launch the user interface. If the user interface does not launch automatically the following screen will appear. Double clicking the TRIDION icon will launch the user interface software.

Figure 4-1 screen showing the Windows CE launch window

3. Once the user interface software has been initiated the instrument pumps turn on to establish vacuum and the heated parts of the instrument begin to increase in temperature. The following screen shows the status of the instrument initializing.

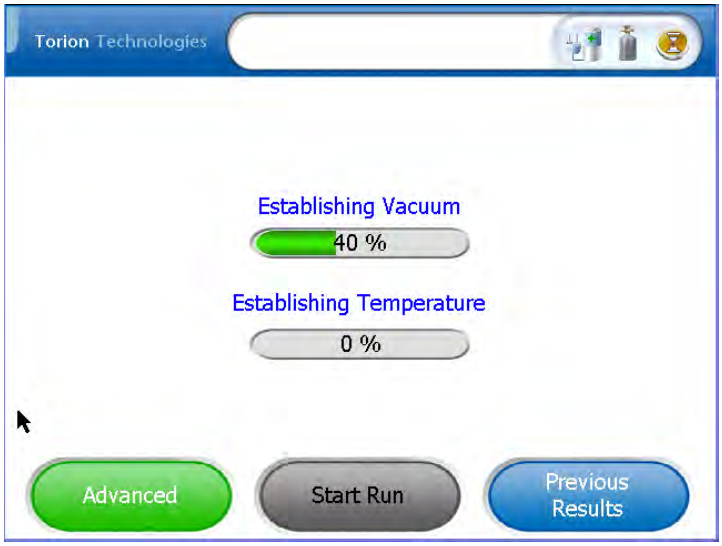


Figure 4-2 Initialization of the instrument

4. The TRIDION is equipped with a touch screen interface. It also has a USB port and a USB mouse can be connected directly to the instrument. The functionality of the touch screen is the same as for a mouse. Touching the screen will select a button and activate the commands associated with the button. Using a mouse to position a pointer over a button and then clicking on the button with the mouse will also activate the command associated with the button.

5. An alternative option to run the instrument directly from a PC is to use tight VNC viewer. Tight VNC viewer is not included with the software, but is available for free downloaded from the internet. Instructions on how to install and use the viewer are included in the Software chapter of this manual.

6. The instrument has a stylus attached to facilitate operation of the touch screen. The location of the stylus is shown in the following image.

Although the flow of this chapter is linear in the way it presents the user interface, any of the buttons that appear either blue or green on any screen can be accessed from that screen. If they are gray then they are disabled. The screens that open are the same regardless of what screen they are accessed from.

Figure 4-3 Instrument Parts

Standard Operating Procedures

1. Once the instrument has established vacuum and proper operating temperatures the screen shown below is displayed, which is Step #1 of the manufacturers Standard Operating Procedures. The instrument functions using Standard Operating Procedures to simplify running the instrument and help prevent user error. The TRIDION-9 comes from the manufacturer with one SOP written that performs the following functions:

    a. Run a system blank
    b. Run a performance validation
    c. Run Samples (up to 20 samples)

2. Once an SOP has finished it starts from the beginning.

3. If users want to create a different SOP they need contact Torion Technologies.

Status bar

1. The top section of most screens on the instrument is the status bar.

2. The status bar contains three icons in the upper right hand corner. The image below shows the status bar displayed.

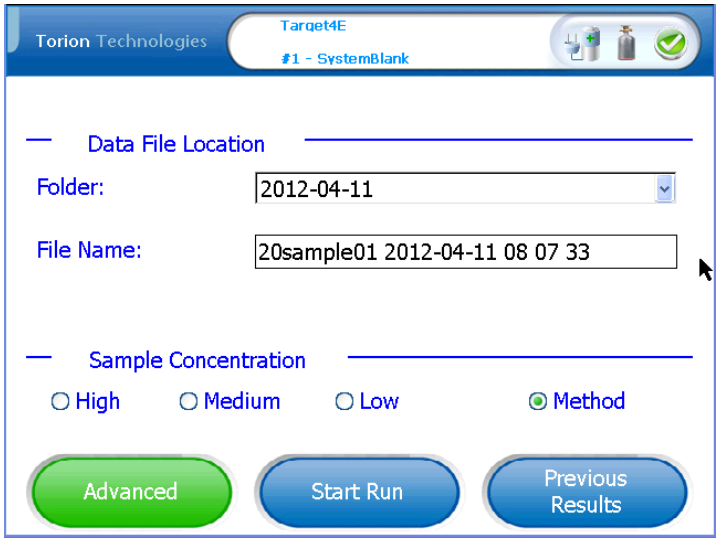


Figure 4-4 Status bar displayed at the top of the screen

3. The icon furthest to the right displays whether the instrument is ready to perform a run. The instrument is ready to run when a green circle with a check mark inside is displayed.

4. The icon in the middle displays the % of helium left in the helium cartridge. If the instrument is attached to laboratory helium the icon will display that the cartridge is empty or have a value of 1%.

5. The icon on the left displays the amount of battery power left, or if the instrument is plugged into AC power.
6. To view the status of the instrument choose any of the icons in the upper right hand corner of the screen and an expanded view of the instrument status will appear as shown in the image below.

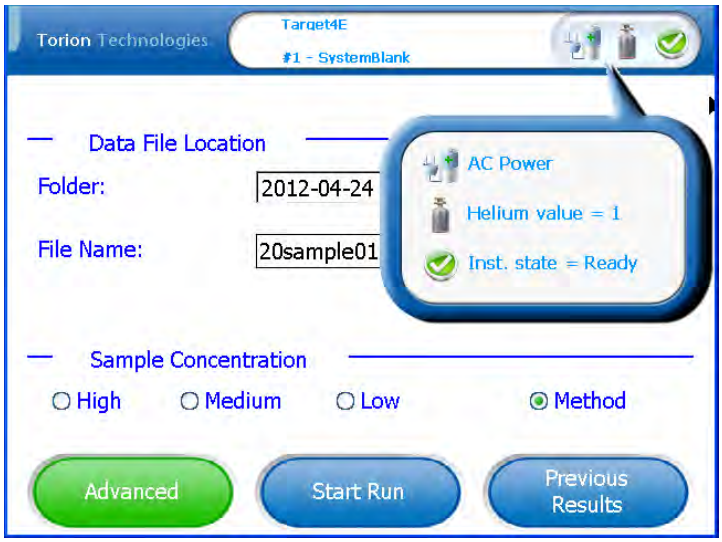


Figure 4-5 Instrument status shown in expanded view

7. In the middle section of the status bar, the name of the activated method is displayed at the top, as shown in the image above. In this example the method name is Target 4E.

8. The type of sample is displayed just below the method name in the status bar, as shown in the image above. In this example the sample type is #1 – SystemBlank.

Running a blank

1. SOP step #1 is to run a system blank. The first screen to appear after the system has reached operating status is shown in the figure below.

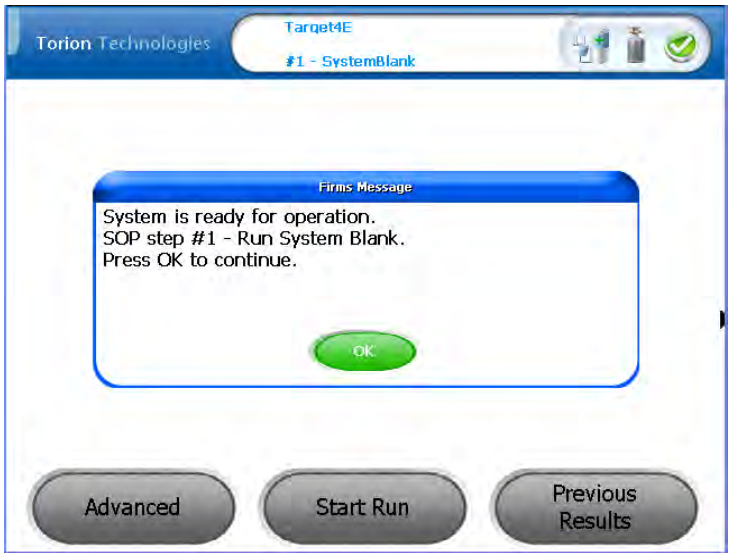


Figure 4-6 SOP step #1 – Run System Blank

2. Selecting the **OK** button prepares the instrument for a system blank and the Home screen appears as shown below.

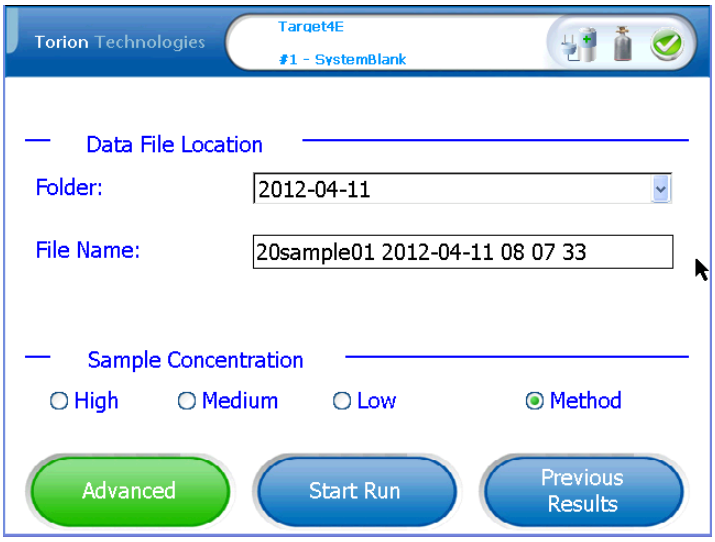


Figure 4-7 Home screen ready to perform System Blank Run

3. Choosing **Start Run** initiates a system blank run after choosing to run a System Blank Run from the previous screen.

4. The following image shows the screen that is displayed after selecting the **Start Run** button.

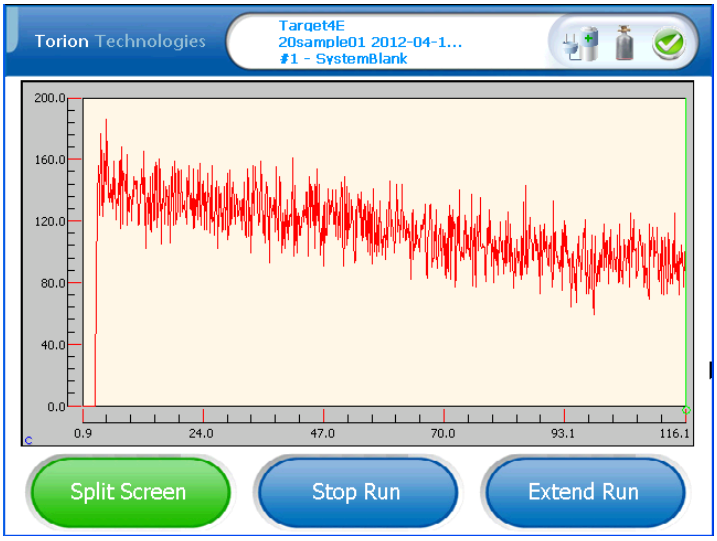


Figure 4-8 System blank screen displayed while running a blank

5. This screen shows a chromatogram of a clean system blank where there are no contaminant peaks.

6. The following image shows the screen that is displayed after the system blank run is finished and the system is processing the run data, looking for any contamination peaks.

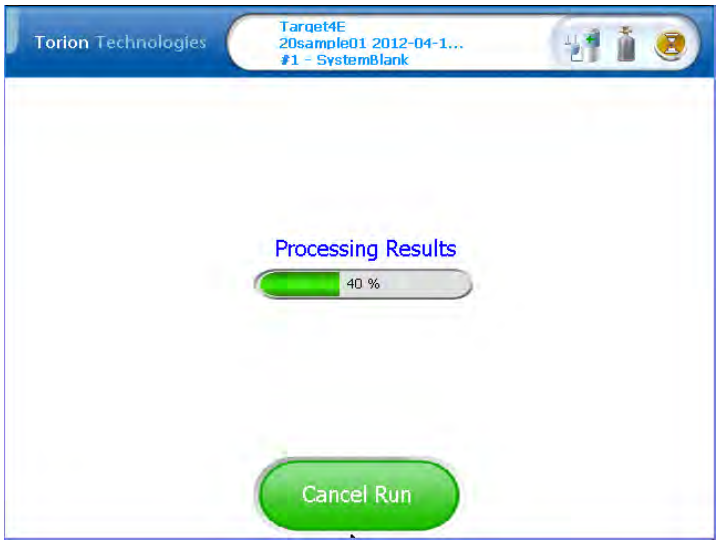


Figure 4-9 Processing Results screen

7. The following image shows the screen that is displayed after the system blank is performed and analyzed. If there were any contaminant peaks, the contaminants might be identified by the on-board instrument library. If any positive identifications were made they would be listed in the identification table at the bottom of the screen.

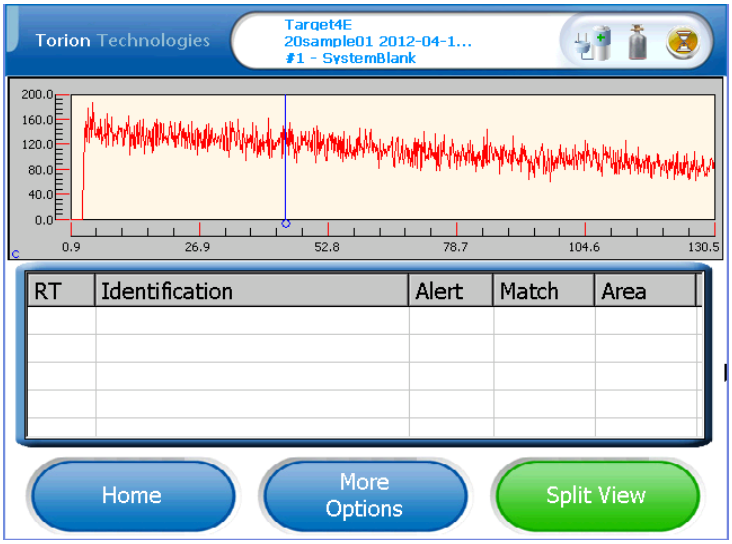


Figure 4-10 Results screen shown after system blank run is performed

8. The following image is an example of a contaminated blank run. As shown in the text at the top of the screen an actual System Blank was run, but there were contaminant peaks. The peaks were either identified or listed as unknown compounds by the library, as shown at the bottom of the screen.

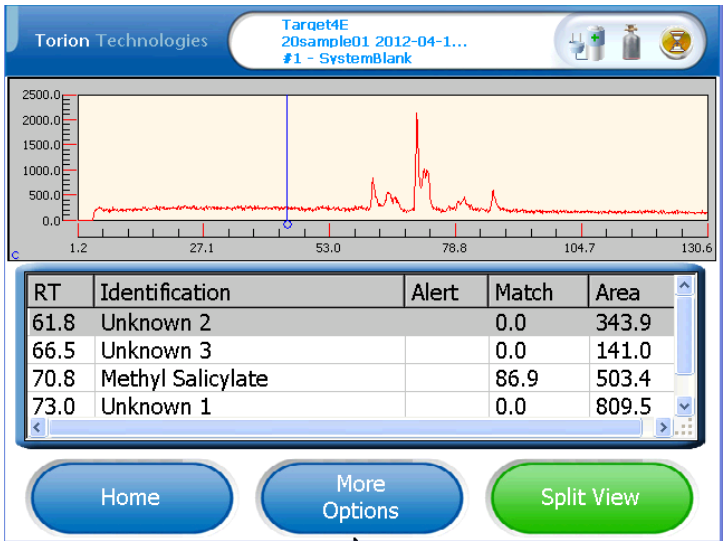


Figure 4-11 Results of a system blank run that contained contaminant peaks

9. From the results screen choose **Home** to continue running the instrument.

10. If the System Blank run was contaminated the following screen appears.

Figure 4-12 Contaminated System Blank run notice

11. The above screen is only shown if there were contaminant peaks found. The user may choose to continue to run the instrument as normal, or choose to perform another blank run. If the user chooses **Yes**, then the same screens as above are displayed on the instrument.

12. If the user chooses **No**, not to perform another System Blank run, or if the System Blank run was clean in the first place, the following screen will appear. The system is now ready to perform SOP step #2.

Running a Performance Validation

1. The second step of the manufacturers SOP is running a Performance Validation.

2. After running a System Blank run the following image shows the screen that is displayed.

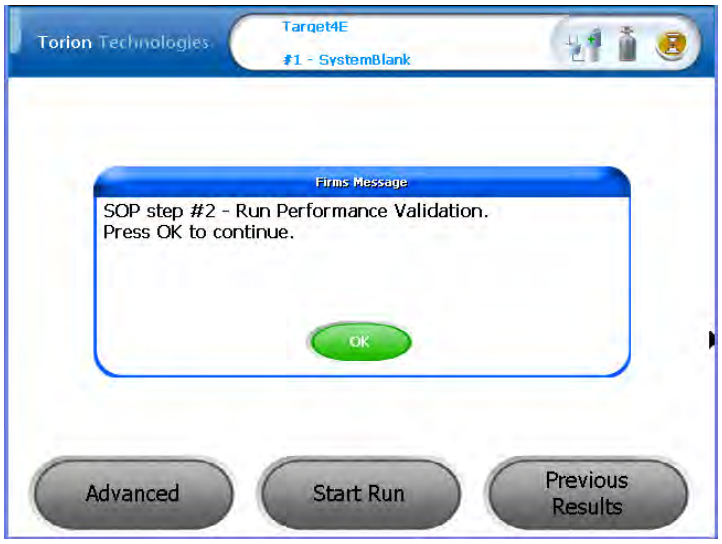


Figure 4-13 SOP step #2 – Run Performance Validation screen

3. Choose **OK** to run a Performance Validation.

4. Sometimes the following screen will appear in between instrument runs. This screen indicates that the instrument is still cooling down the GC column back to the initial set point before the next run can be performed.

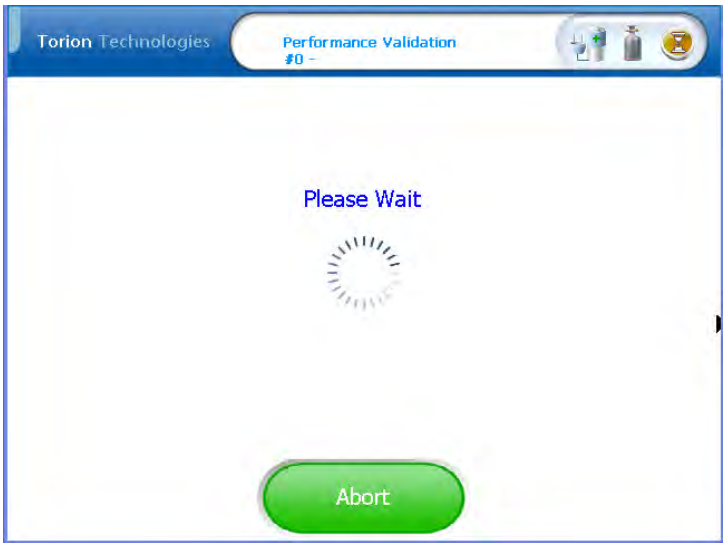


Figure 4-14 Please Wait screen indicating that the GC column is still cooling to initial set point

5. Once the instrument is ready to perform the next run the following screen will appear, prompting the user to insert the syringe and depress the plunger.

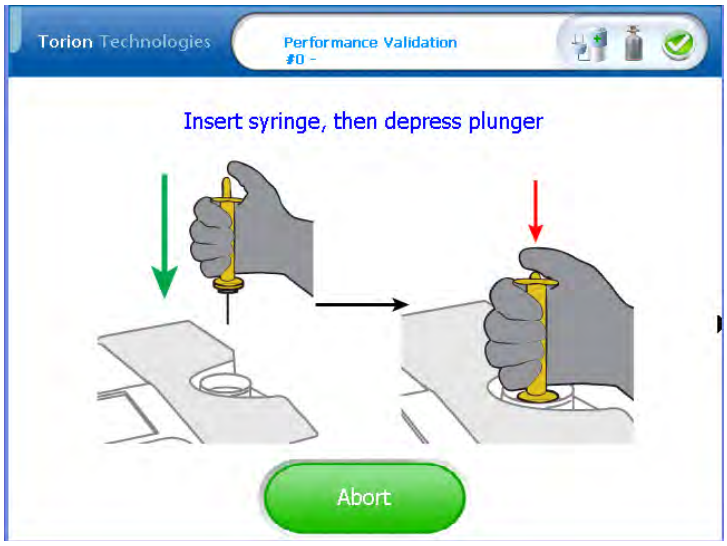


Figure 4-15 Instructions on how to perform an injection

6. The following image shows the screen indicating for the user to wait while the analytes thermally desorb from the SPME fiber into the GC injection port.

Figure 4-16 Please wait injection screen

7. The following image indicates when the user should depress the plunger of the CUSTODION syringe and remove the syringe from the GC injection port.

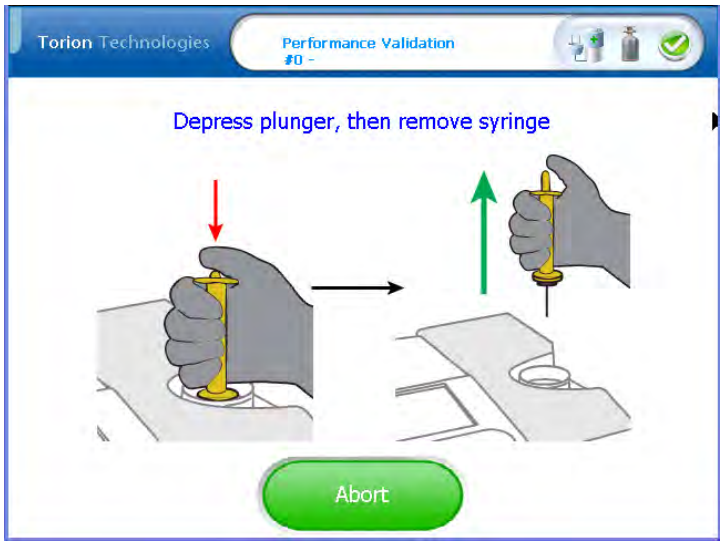


Figure 4-17 Depress plunger, then remove syringe screen

8. The following image shows the screen that is displayed while the system is running a performance validation.

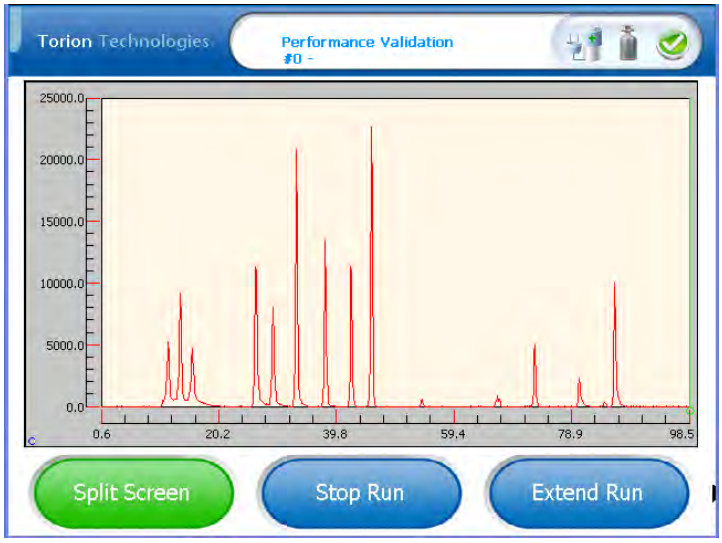


Figure 4-18 Screen shown while running a Performance Validation

9. The following image shows the screen that is displayed when the calibration succeeds.

Figure 4-19 Calibration Succeeded

10. The following image shows the screen that is displayed if the calibration fails.

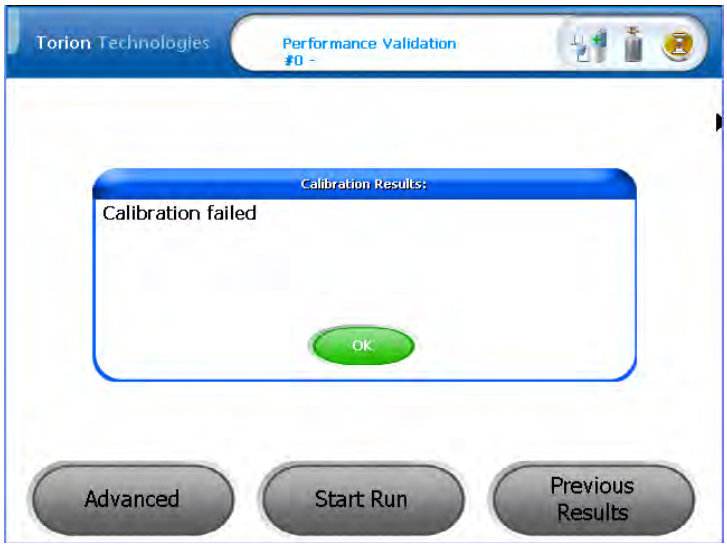


Figure 4-20 Calibration results screen when calibration fails

11. After choosing **OK** the following screen appears to retry the performance validation.

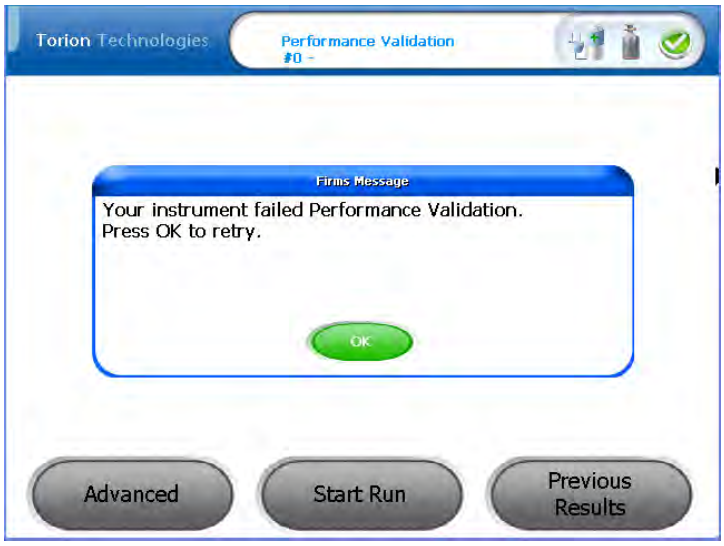


Figure 4-21 Retry Performance Validation

12. After choosing **OK** the instrument screens prompt the user to perform an injection as shown previously.

13. The following image is shown when the calibration succeeds.

Figure 4-22 Calibration results screen when calibration succeeds

14. Choose **OK** to proceed.

Running Samples

1. The third step of the manufacturers SOP is running samples.

2. The following screen indicates that the instrument is now ready to run samples.

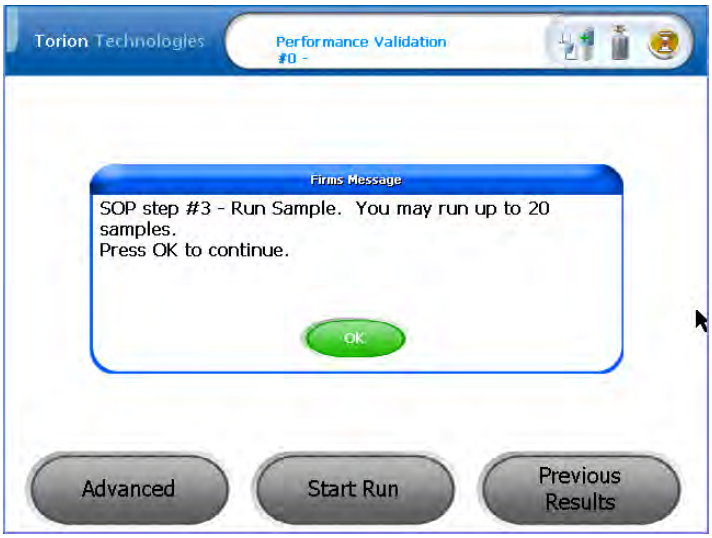


Figure 4-23 SOP step #3, instrument is ready to run samples

3. Choose **OK** to proceed and start running samples.

4. The following image shows the home screen that is displayed when the instrument is ready to perform sample analytical runs.

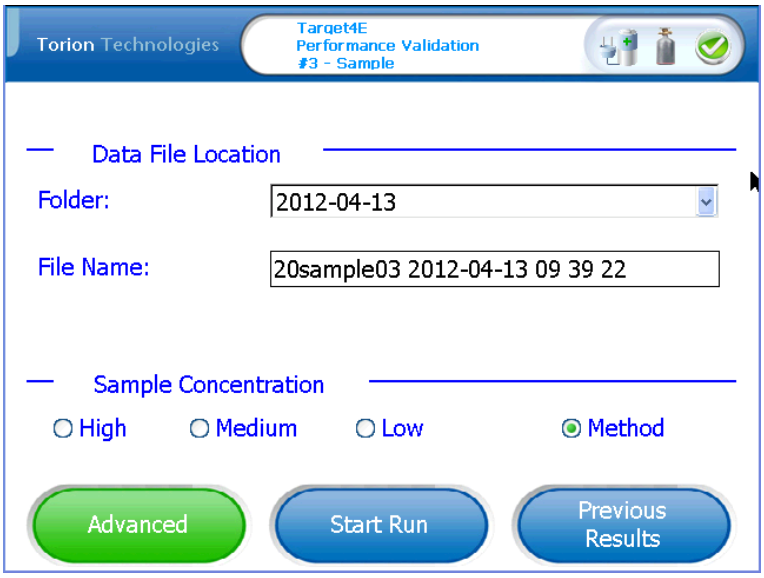


Figure 4-24 Home screen ready to run samples

Data File Names

1. For every run the instrument automatically creates a file name as displayed in the image above. Users may change this name before starting a run.

2. To change the file name highlight the **File Name:** field and an alphabet touch board will appear on the screen. The user can start typing the new run name.

3. The instrument also automatically creates a data folder for each day. All run data is stored in the daily folder. The user may choose a different folder for run data to be stored in.

4. To change the data storage folder touch the drop down arrow in the **Folder:** field and highlight the desired folder.

Sample Concentration

1. When the instrument is being run the split flow settings in the GC method are used automatically. Occasionally users may come across samples with very low concentrations to very high concentrations where the split flow should change, but the user does not want to restart the SOP in order to change the method. In this case the user may choose an appropriate sample concentration which will change the split flow without interrupting the SOP.

2. From the home screen as shown in the above image, a user would choose the following Sample Concentrations to have the following effect on the Split Flow:

   High - opens both the 10 ml and 50 ml split valves
   Med - opens the 10 ml and closes the 50 ml split valves
   Low - closes both the 10 ml and 50 ml split valves
   Method - follows the activated GC method settings

3. Choose **Start Run** to begin the run.

4. Once the user chooses **Start Run** the screens prompt the user to perform an injection as shown previously in this section. The injection screens are the same as when running a performance validation.

5. The following image shows the screen that is displayed during a sample run.

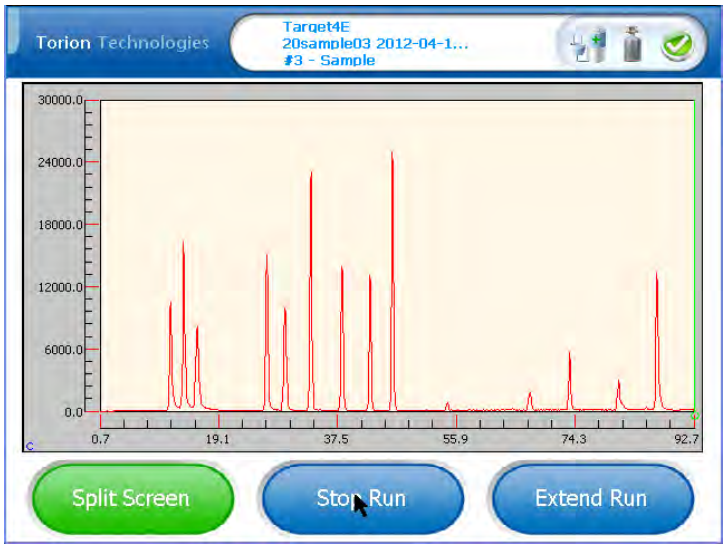


Figure 4-25 Screen shown during a sample run

6. The following image shows the screen that is displayed when the **Split Screen** option is selected from the run screen.

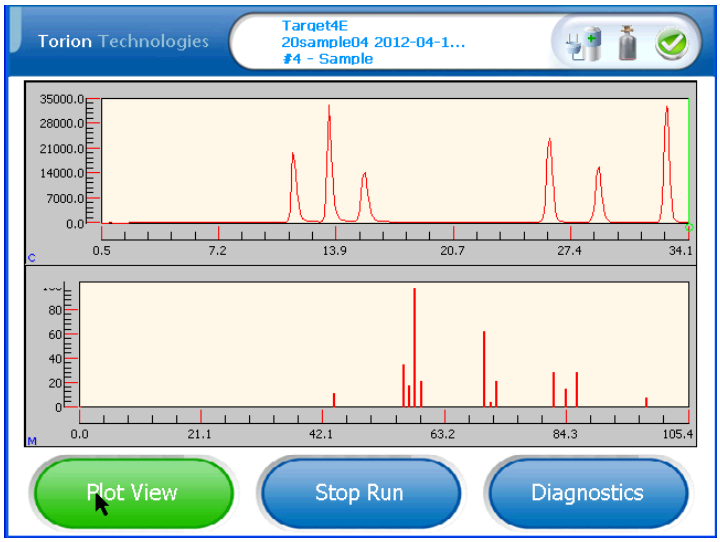


Figure 4-26 Screen shown during a run using the Split Screen

7. With the **Split Screen** option selected during a run the total ion chromatogram (TIC) is plotted at the top of the screen and the mass spectra are shown on the bottom plot. The spectra plot shows the most recently collected spectra unless the cursor is positioned at a specific scan location earlier in the TIC plot. In that case the spectra displayed in the spectra window correspond to the selected scan in the TIC plot.

8. Selecting the **Plot View** option will return the screen to displaying chromatographic data only.

9. Selecting the **Stop Run** button stops the analysis and the screen changes to an intermediate screen. The intermediate screen is shown at the end of any run while they system is returning to a ready state. The intermediate screen is described later in the chapter.

10. The **Diagnostics** button opens the Status/Diagnostics screens that are described later in this chapter.

11. On the touch screen data, the user can drag a square around a section to zoom in on. The following image shows the screen as a square is being dragged around a section to zoom in on.

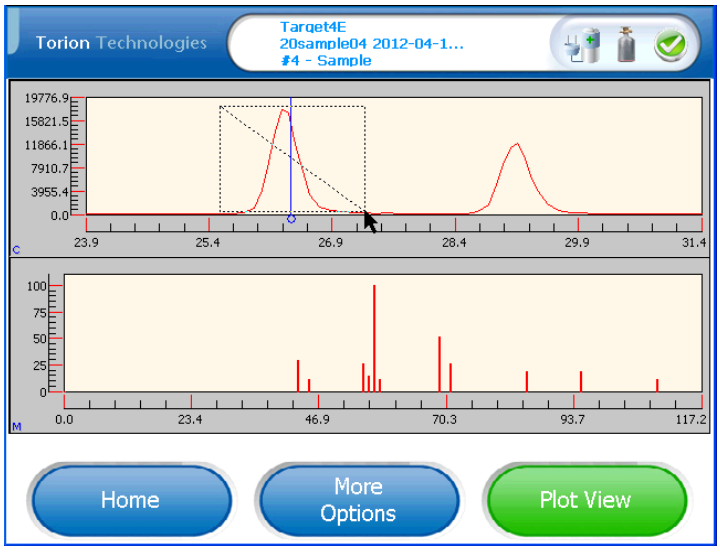


Figure 4-27 Screen showing Zoom feature in the TIC window post run

12. The following image shows the library results screen displayed a the end of a run.

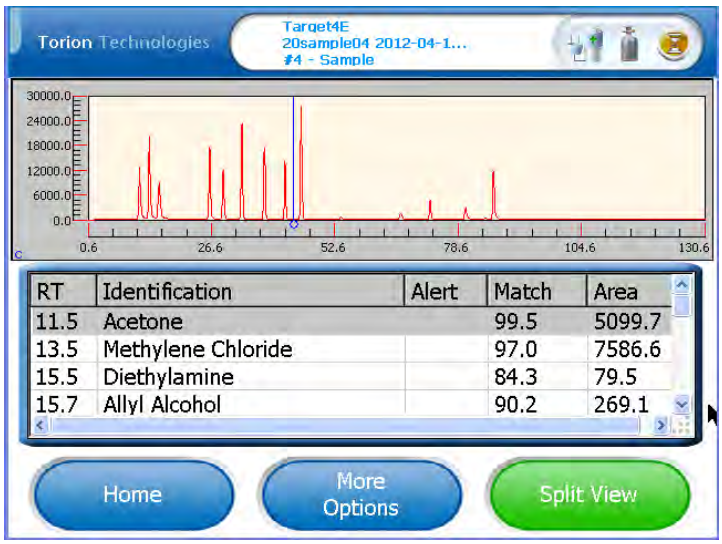


Figure 4-28 Library results screen shown at the end of a run

13. In the figure above, the table on the bottom of the screen shows the post run results table, or the library hits. See the Run a Sample section of this manual for a detailed description of the table. The zoom features works the same during a run as it does post run.

14. The following image shows the screen that is displayed after choosing the **Split View** option and using the zoom function on the TIC plot.

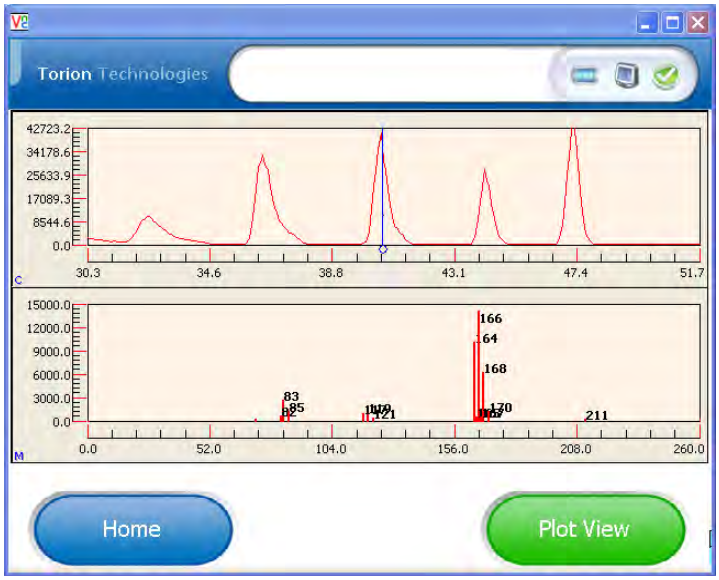


Figure 4-29 Screen showing the zoomed in results with Split View showing spectra at cursor position

15. The spectra of a specific scan can be previewed by placing the cursor at the desired scan in the TIC plot at the top of the screen. To place the cursor, simply touch the screen at the location where the cursor should be placed.

16. The following image shows the screen that is displayed while using the zoom function in the spectra plot.

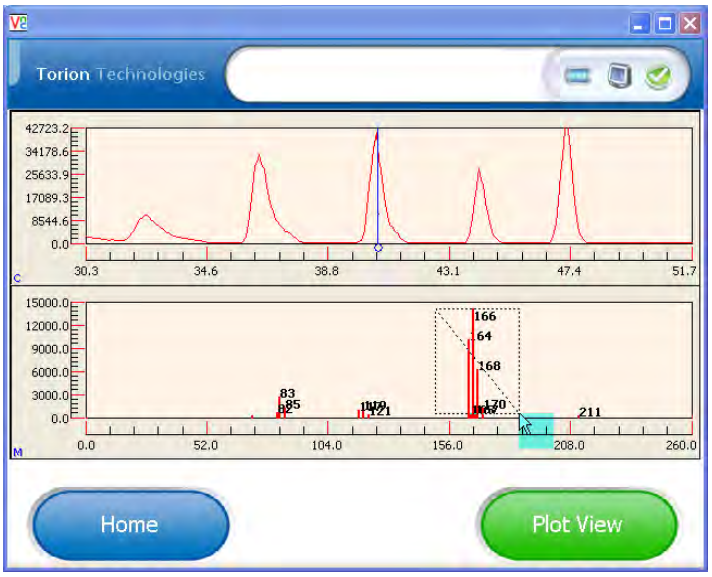


Figure 4-30 Screen showing the zoom function in the spectra window

17. The following image shows the screen that is displayed after using the zoom function in the spectra plot.

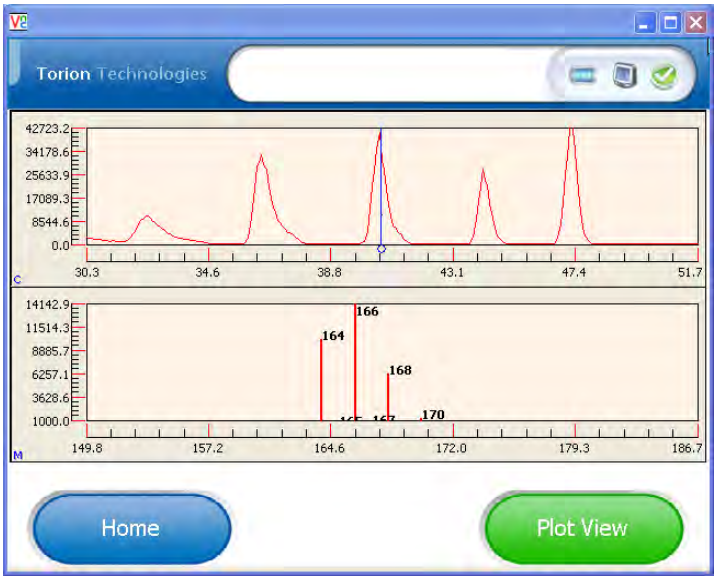


Figure 4-31 Screen showing the zoomed in section of the spectra window

18. The following image shows the screen that is displayed when zooming out in TIC plot.

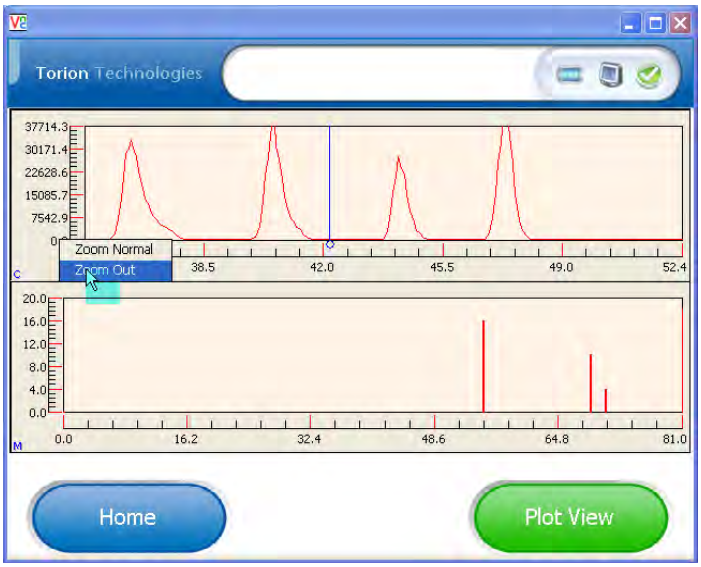


Figure 4-32 Screen showing the zoom out function

19. To zoom out in either the TIC plot or the spectra plot, select the bottom axis area of the plot with the stylus. The box will open with the option to **Zoom Normal** or **Zoom Out**.

20. **Zoom Normal** restores the full view of the TIC plot or the spectra plot depending on which plot axis was selected.

21. **Zoom Out** returns to the view to the last zoom selection. If the user has zoomed in twice the view returns to the first zoomed in view.
22. Selecting the **Home** button returns the screen to the next step in the SOP.

23. Once the instrument has finished the entire SOP the following screen will appear.

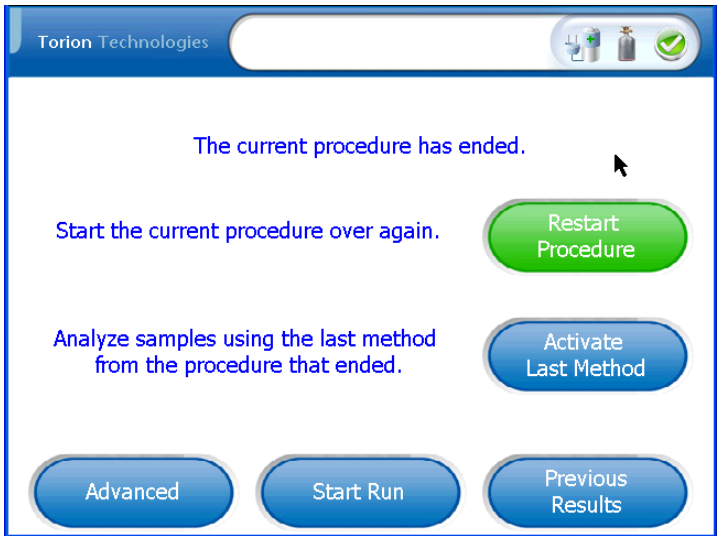


Figure 4-33 Current procedure has ended screen

24. Selecting **Restart Procedure** will start the SOP from the beginning with first running a System Blank.

25. Selecting **Activate Last Method** will allow the user to run samples on the instrument using the last GC method. This bypasses having to re-run a System Blank or Performance Validation prior to running samples.

26. Selecting **Advanced** or **Previous Results** will move to these functions within the user interface, which are discussed in detail in the following sections.

Advanced

1. Pressing the **Advanced** button from any screen within the user interface displays the following screen.

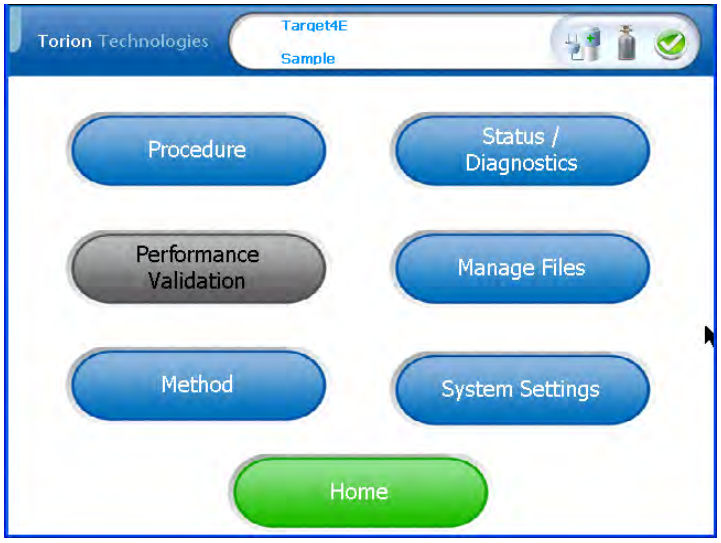


Figure 4-34 Advanced screen

Procedure Button

1. The **Procedure** button will be used to select and load various SOPs.

Status/Diagnostics Button

1. Selecting the **Status/Diagnostics** button opens the following screen.

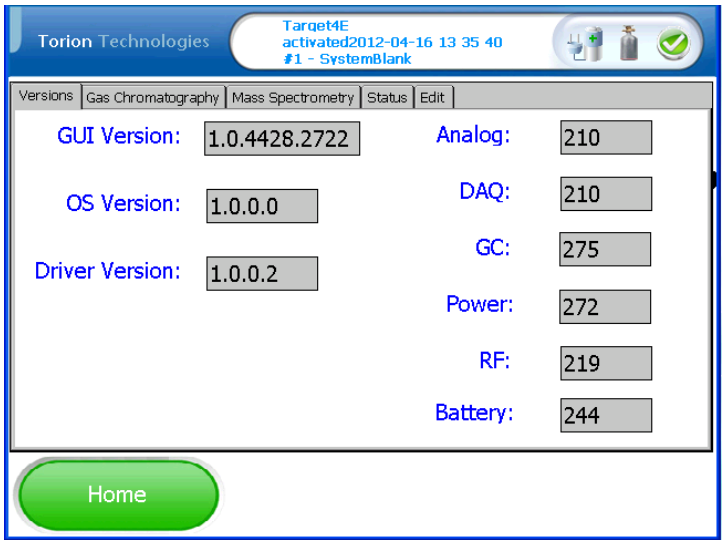


Figure 4-35 Version tab of the status diagnostics screen

2. With the **Versions** tab selected this screen shows all of the information about the versions of code used in the instrument. This information is used by service personnel to ensure that all of the correct control software has been loaded onto the instrument.

3. Selecting the **Gas Chromatography** tab opens the following screen.

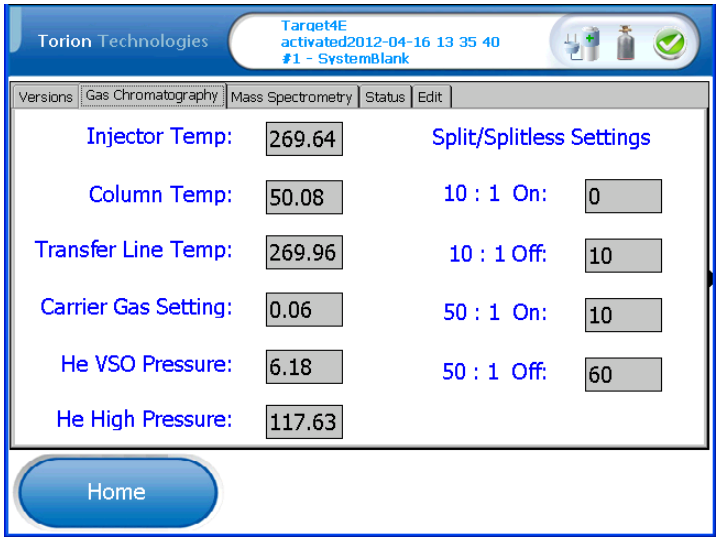


Figure 4-36 Gas Chromatography tab of the Status/Diagnostics screen

4. This tab shows the actual temperatures and pressures of the various components of the GC. It also shows the Split/Splitless Settings.

5. Selecting the **Mass Spectrometry** tab displays the following screen.

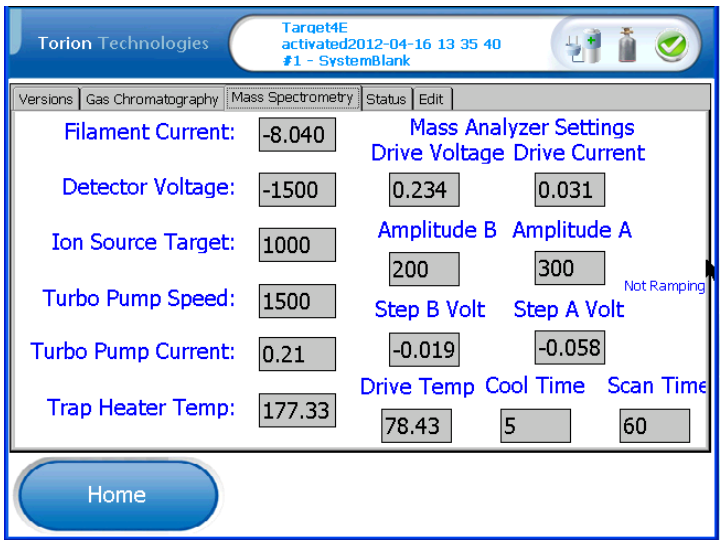


Figure 4-37 Mass Spectrometer tab of Status/Diagnostics screen

6. This screen shows actual values from the mass spectrometer. These values are used by service personnel to diagnose potential problems with the instrument.

7. Selecting the **Status** tab displays the following screen.

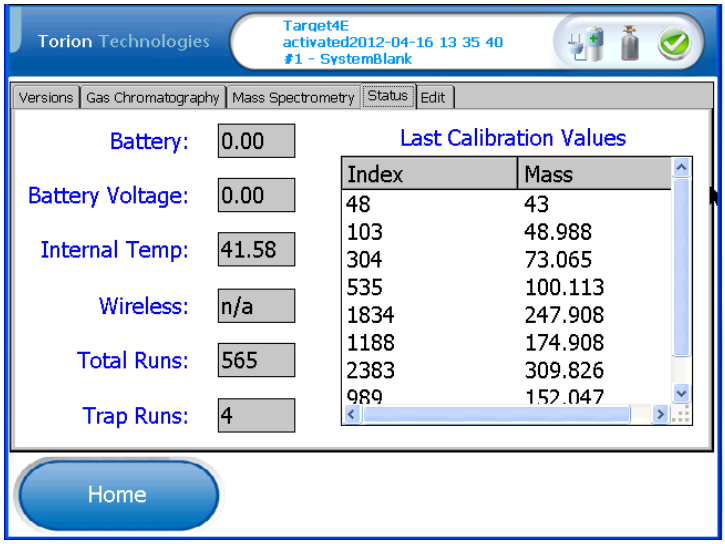


Figure 4-38 Status tab of the Status/Diagnostics screen

8. This screen shows the percent of **Battery** life remaining, **Internal Temperature** of the system, **Wireless** status, **Total Runs**, and the number of **Trap Runs** on the instrument since the trap was last cleaned.

9. The following image shows the **Edit** tab screen.

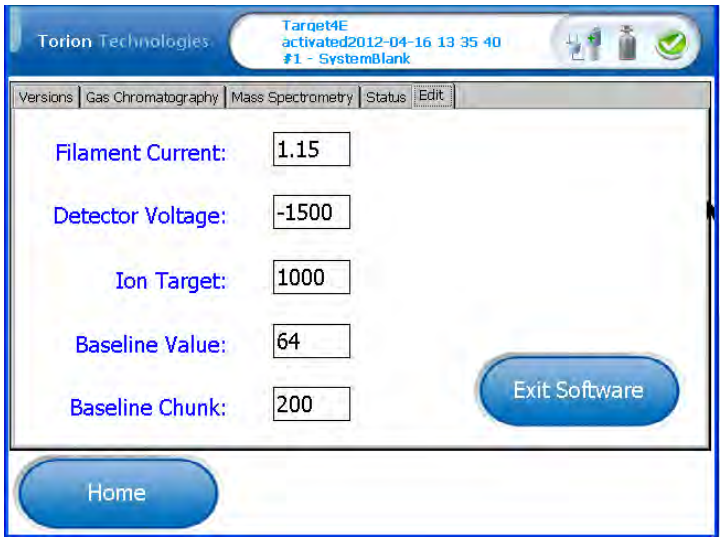


Figure 4-39 Edit tab of the Status/Diagnostics screen

10. On this screen the user can manually set the Filament Current, Detector Voltage and the Ion Target by touching the desired field with the stylus. In future releases other parameters that deal with the GC will also be editable from this screen.

11. To edit any of the parameters touch the box containing the setting and the following screen will appear where the users will have to enter a password.

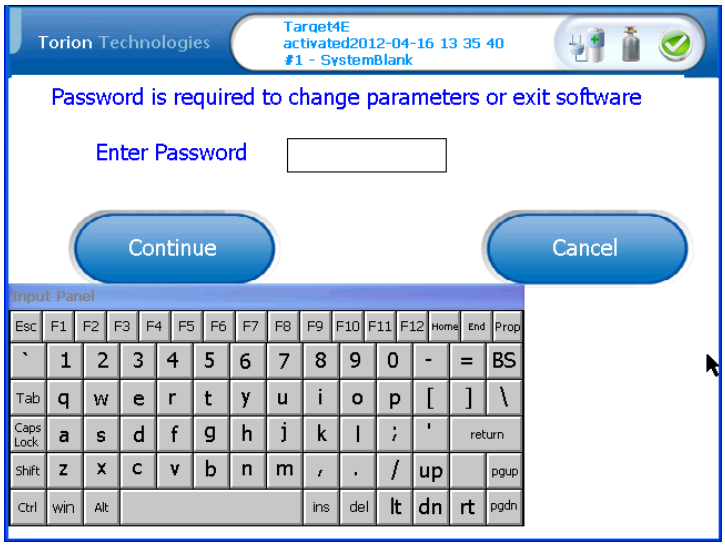


Figure 4-40 Enter Password screen

Caution!

These changes take effect immediately (even in the middle of a run) and should only be adjusted by experienced users. The changes are not saved in the method and will be replaced as soon as a new method is loaded into the instrument. If it is desired to keep the changed parameters it will be necessary to modify a method file in the CHROMION software and load the saved method as the active method.

Manage Files Button

1. The following screen opens after selecting the **Manage Files** button. The Manage Files tool is used to rename, delete or copy files from the SD Memory Card on the instrument to a USB memory stick.

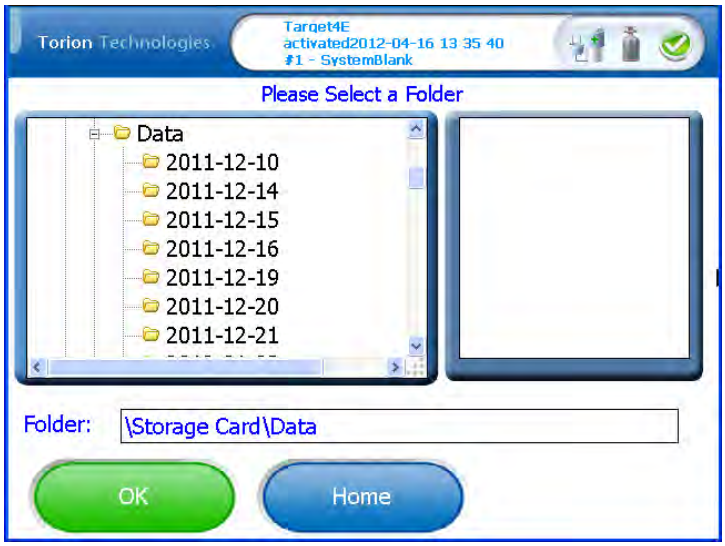


Figure 4-41 Screen that is displayed after selecting the manage files from the advanced screen

2. Highlight any folder by touching the folder name on the screen with the stylus and choose **OK**.

3. The following screen will appear that lists all of the files within the folder selected in the previous step.

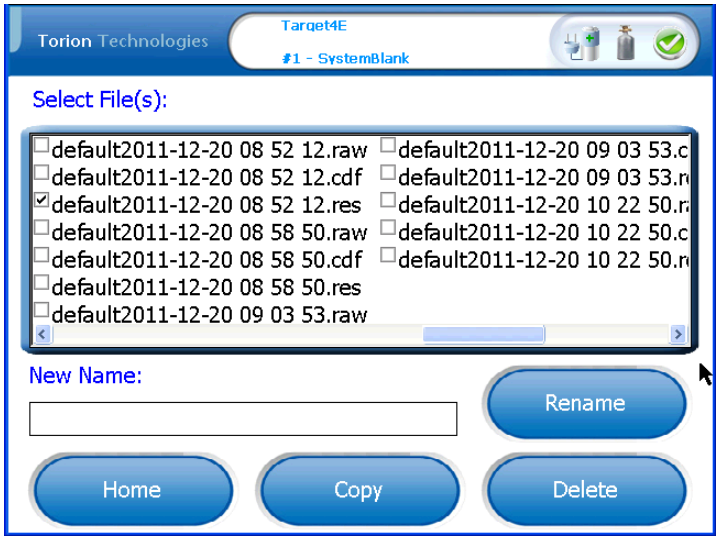


Figure 4-42 Select file(s) to be managed

4. Individual files can be either selected or deselected by touching the check box next to the file name.

5. After selecting the desired files choose to **Rename**, **Delete** or **Copy** the files. The copy function has not yet been activated.

6. Selecting the **Home** button will return the display to the Home screen.

Methods Button

1. The following image shows the screen that is displayed after selecting the **Methods** button from the Advanced screen. From the Methods screen users can select a method to activate, or simply view the method parameters in a selected method.

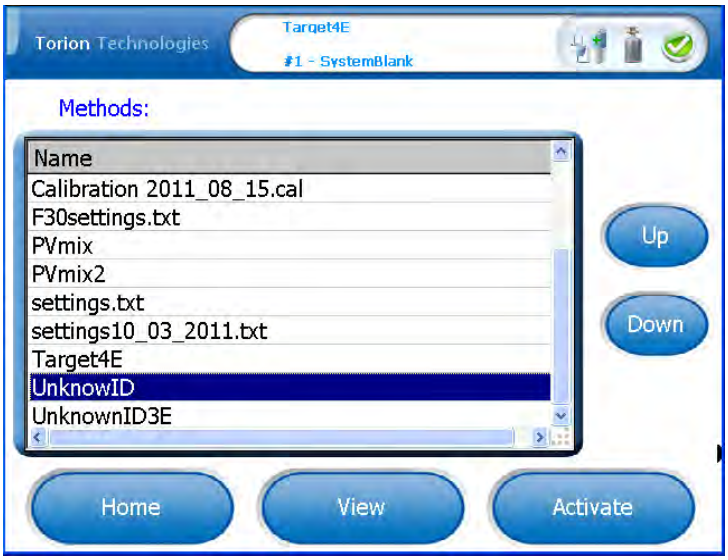


Figure 4-43 screen showing methods selection menu

2. To choose a method, select it from the list by touching it to highlight it.

3. The user can move through the method list by either using the arrows and sliders on the edge of the method window or by using the **Up** and **Down** buttons.

4. Pressing the **Activate** button will make the selected method the active method that the instrument will use for future runs.

5. Selecting the **View** button will open a window as shown below, which displays the settings in the method.

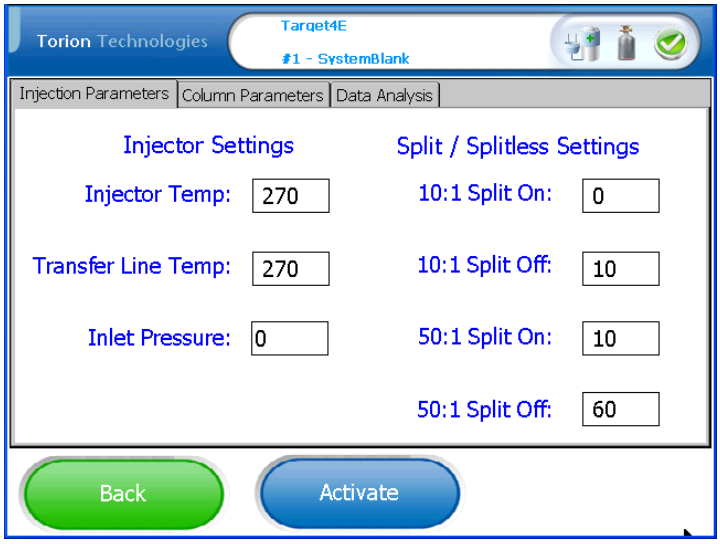


Figure 4-44 Viewing method injection parameters

6. The first tab inside the Methods View screen is the Injection Parameters tab as shown above. This screen displays the method settings for the Injector and the Split Flow.

7. Choosing the **Back** button will take the screen back to the Method screen.

8. Choosing the **Activate** button will activate the method that is being displayed.

9. Choosing the **Column Parameters** tab will display the Column Parameters tab as shown in the figure below.

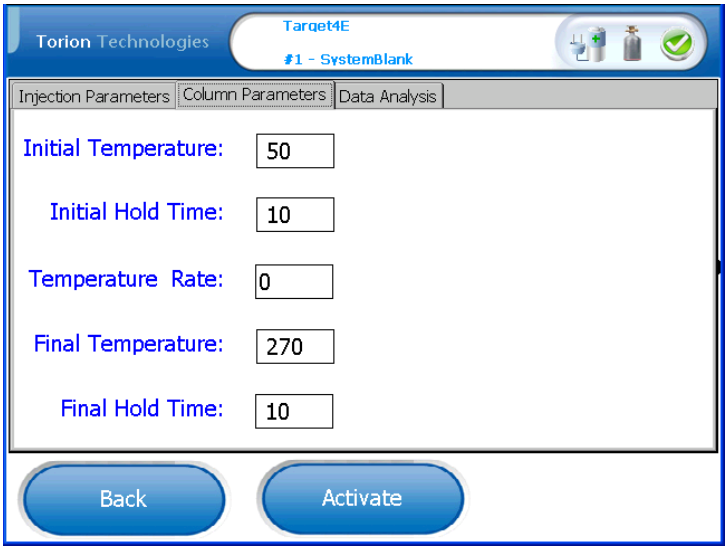


Figure 4-45 Viewing method column parameters

10. The Column Parameters tab displays the set column parameters in the chosen method.

11. Choosing the Data Analysis tab will display the Data Analysis tab as shown in the figure below.

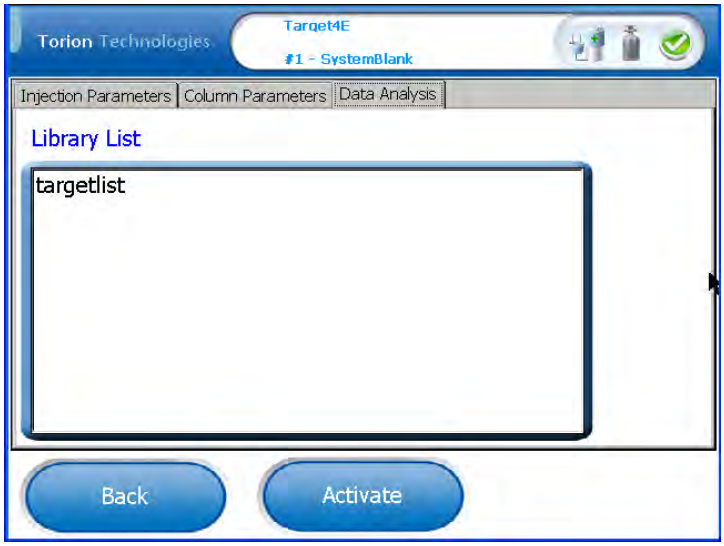


Figure 4-46 Viewing attached library to chosen method

12. The Data Analysis tab displays the name of the library that is part of the selected method.

System Settings Button

1. The following image shows the screen that is displayed after selecting the **System Settings** button from the Advanced screen.

Figure 4-47 Screen showing the system setting options

2. The following image shows the screen that is displayed after selecting the **Set Date / Time** button from the System Settings screen.

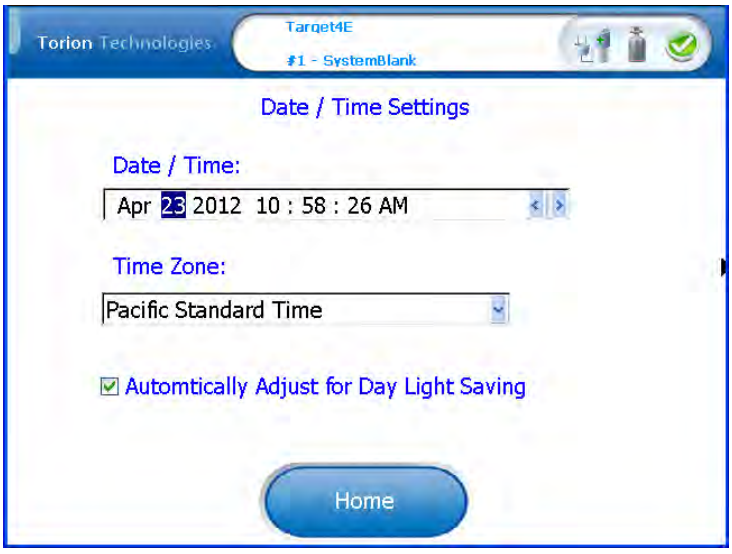


Figure 4-48 screen showing the date and time settings

3. To change the date or time touch the part of the date or time you want to change. The above image has the day selected. Use the arrow buttons on the right of the Date / Time field to change the value.

4. Select a time zone by touching the down arrow on the right side of the Time Zone field and selecting the right time zone from the list.

5. Set day light savings time by touching the button to the right of **Day Light**. The value will switch between Yes and No.

6. Selecting the **Home** button will return the display to the Home screen and will save the Date / Time Settings.

7. The following image shows the screen that is displayed after selecting the **Password** button on the System Settings screen.

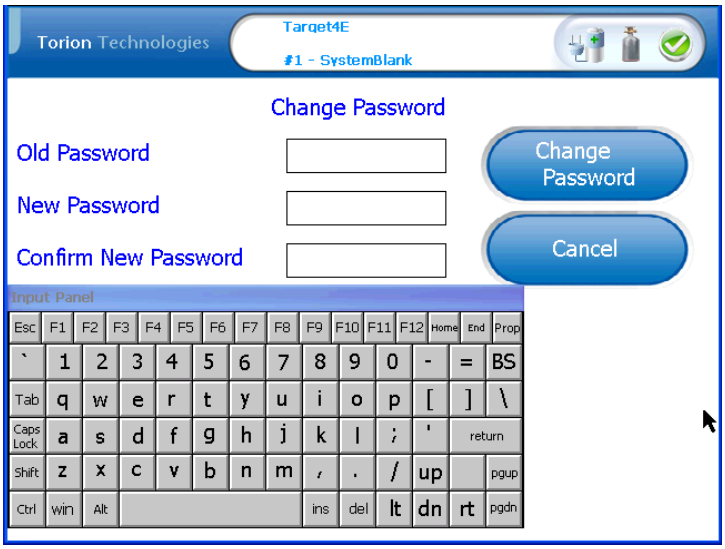


Figure 4-49 Screen showing the password setting screen

8. This screen is used to change the system password.

9. The following image shows the screen that is displayed after selecting the **Update Firmware** button on the System Settings screen.

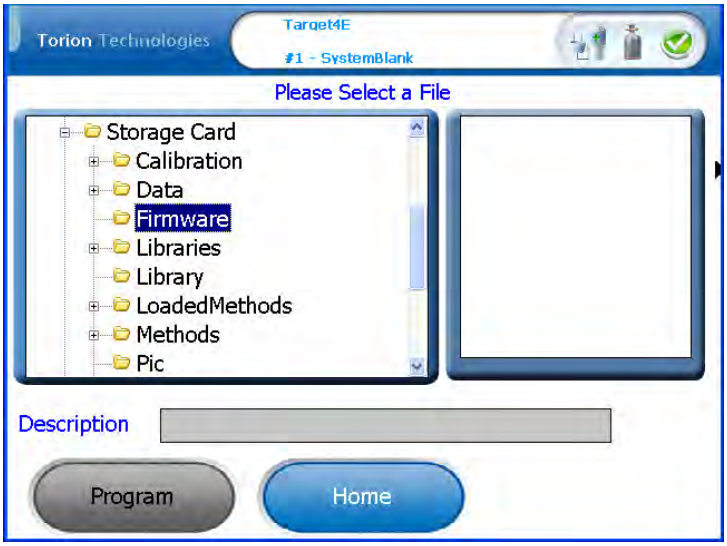


Figure 4-50 Firmware updating screen

10. When updating any Firmware on the instrument a Torion Service Technician will give the user step-by-step instructions at the time of the update.

11. The following image shows the screen that is displayed after selecting the **Install Update** button on the System Settings screen.

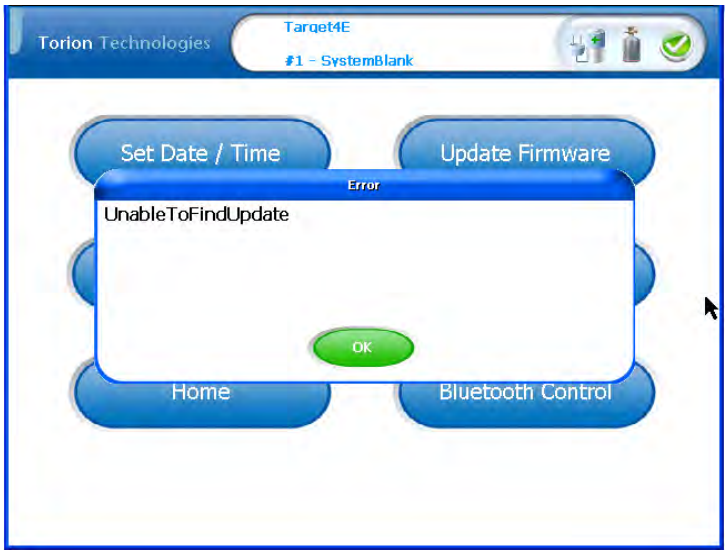


Figure 4-51 Install update error screen

12. When updating any Firmware on the instrument a Torion Service Technician will give the user step-by-step instructions at the time of the update.

13. The following image shows the screen that is displayed after selecting the **Bluetooth Control** button on the System Settings screen.

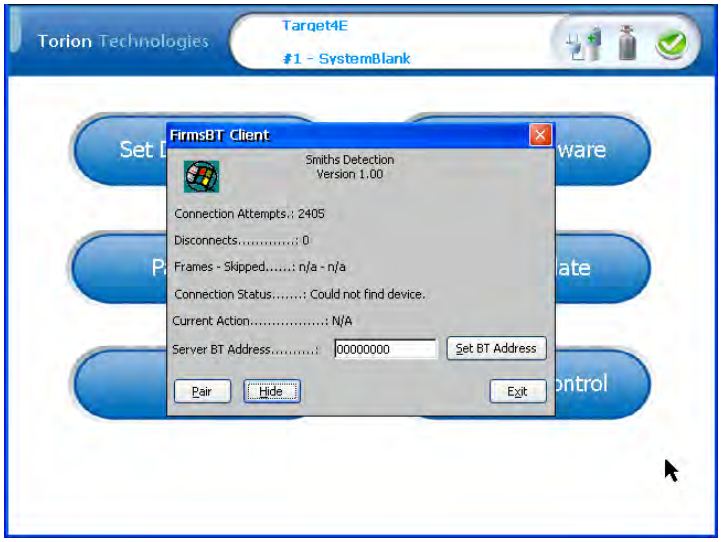


Figure 4-52 Bluetooth control screen

14. Use this screen to input any settings when using a Bluetooth device with the instrument.

Previous Results

1. Pressing the Previous Results button from the Home screen will display the following screen.

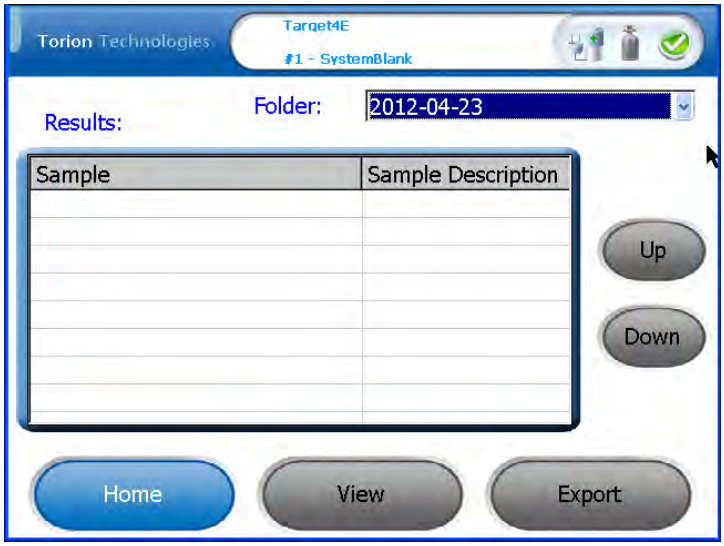


Figure 4-53 Previous Results screen

2. From the Previous Results screen touch the drop down arrow on the Folder list to display a list of folders on the SD card as shown below.

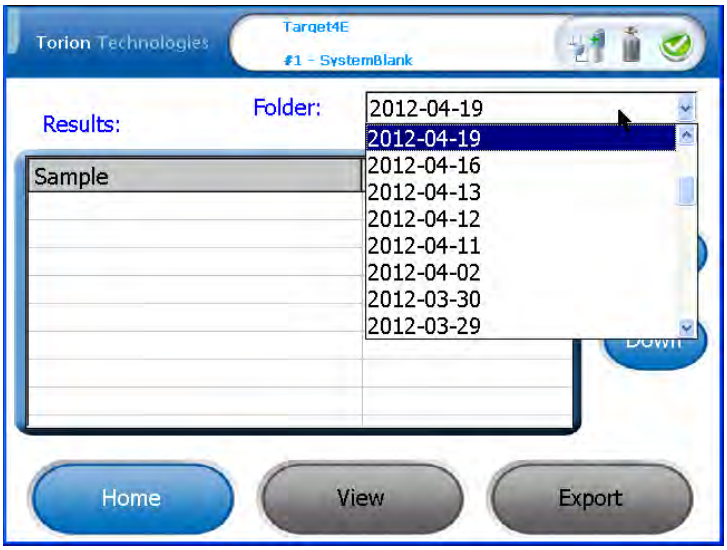


Figure 4-54 Choosing a folder from the Previous Results screen

3. Highlight and double-touch the desired folder. A list of all the data files within the chosen folder will be displayed as shown in the following figure.

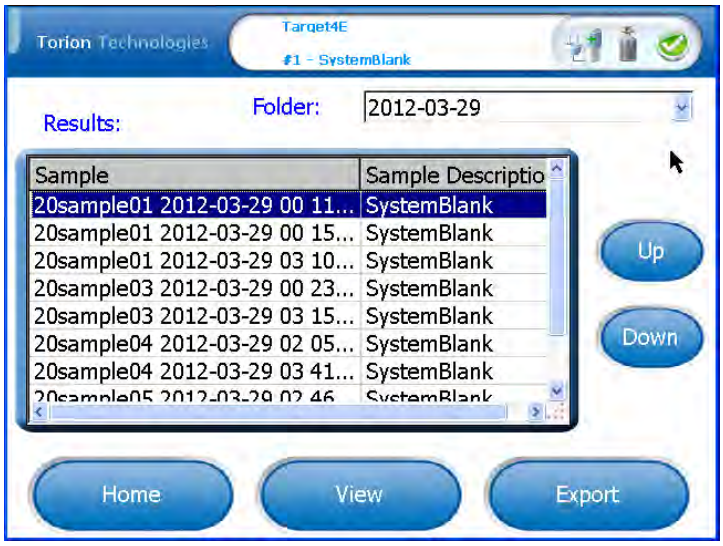


Figure 4-55 Choosing a data file to view previous results

4. To choose a data file, select it from the list by touching it to highlight it.

5. The user can move through the Results list by either using the arrows and sliders on the edge of the results window or by using the **Up** and **Down** buttons.

6. Choose the View button to view on the instrument the results of the data file. The following screen is displayed while the instrument loads the data file.

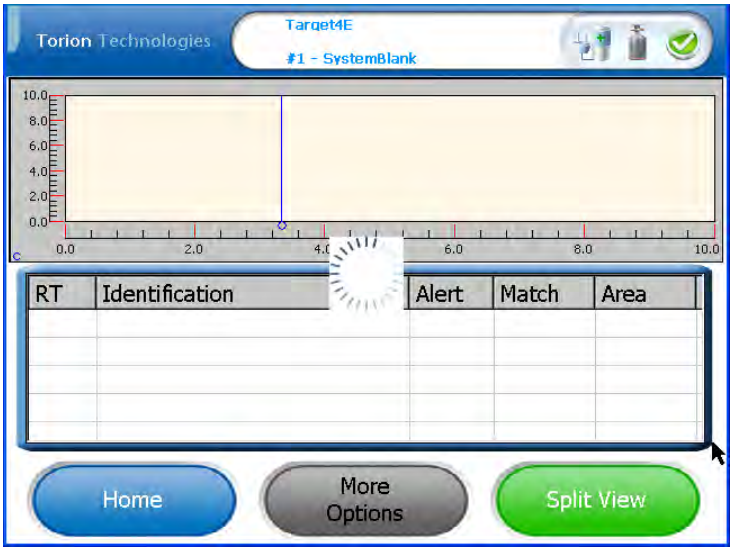


Figure 4-56 Wait screen while instrument processes previous data

7. The following screen is displayed once the data file has been loaded onto the instrument.

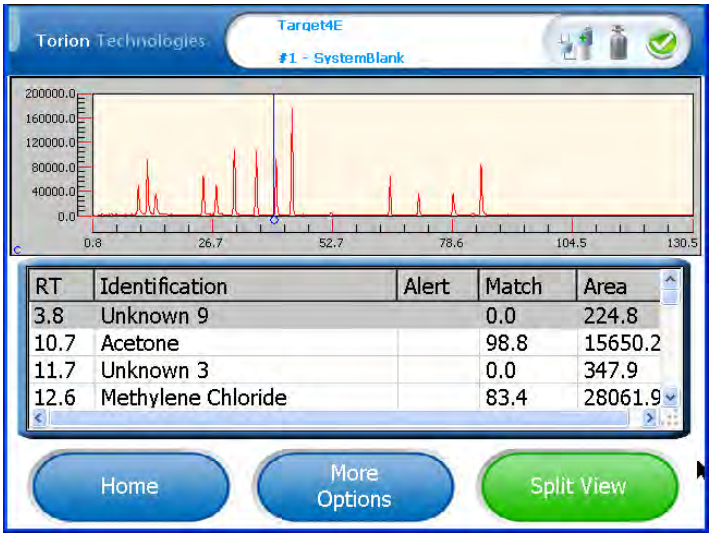


Figure 4-57 Previous data displayed with library identification table

8. The same data is displayed as when the analytical run was processed the first time.

Export Files

1. There are two ways to export files from the instrument SD card to a USB storage device.

2. From the Home screen choose the **Previous Results** button, and then choose the **Export** button. The following screen will be displayed.

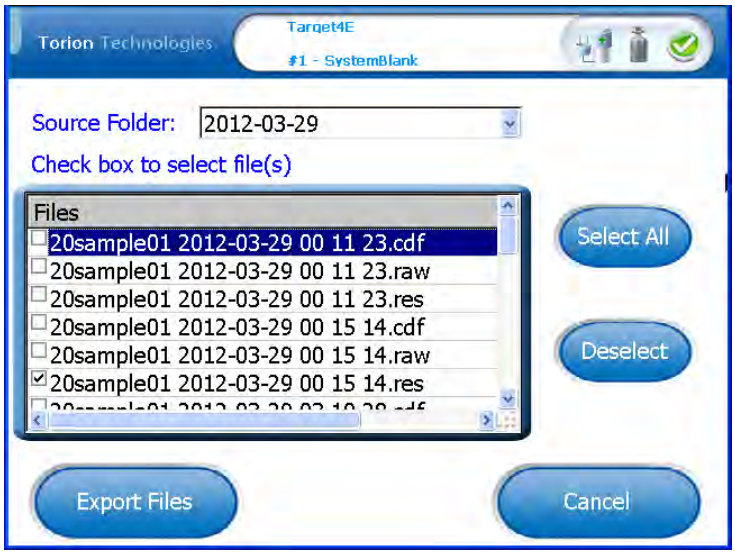


Figure 4-58 Export Files screen

3. To choose a data file, select it from the list by touching the box on the left to place a check in the box.

4. The user can move through the list by using the arrows and sliders on the edge of the window.

5. The user can select or deselect all of the data files by using the corresponding buttons on the right of the screen.

6. Once one or more files have been selected choose the **Export Files** button and the following screen will be displayed.

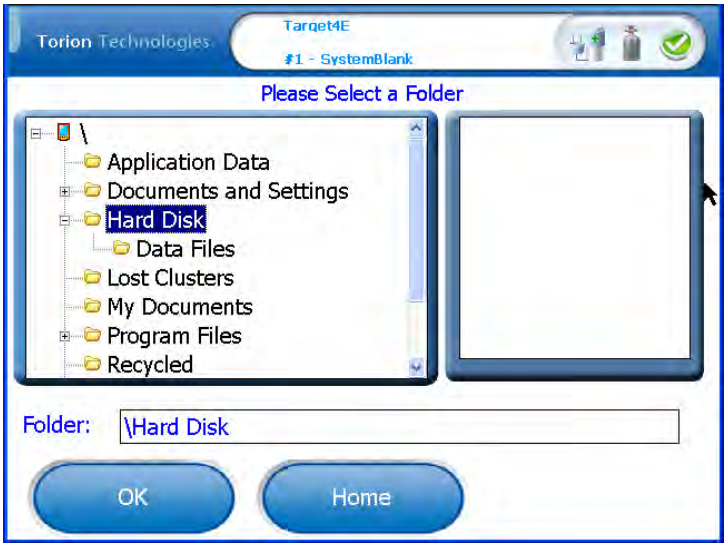


Figure 4-59 Selecting where to export files to

7. A Windows directory is displayed on the left. The user should navigate to and highlight the location where the data files will to be exported to. The Hard Disk is the storage device plugged into the USB port. Choose **OK** to export the data files.

8. When the data files have successfully been exported the following screen will be displayed.

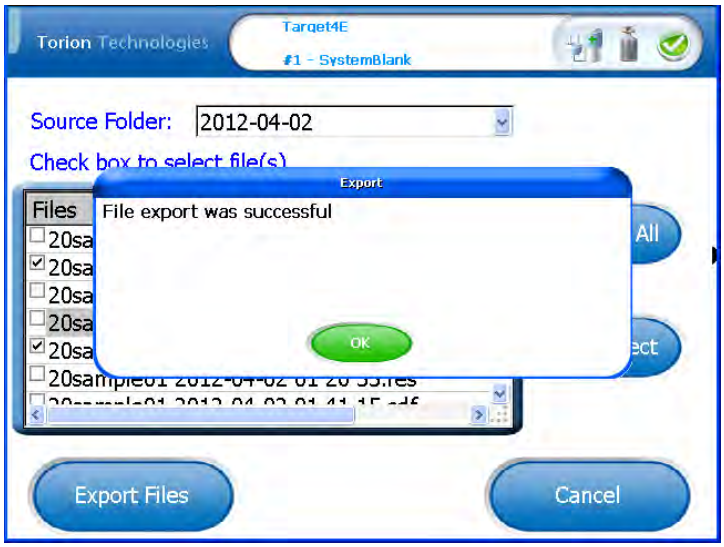


Figure 4-60 File export was successful

9. The Export Files function can also be accessed from the screen displaying end of run data shown in the following figure.

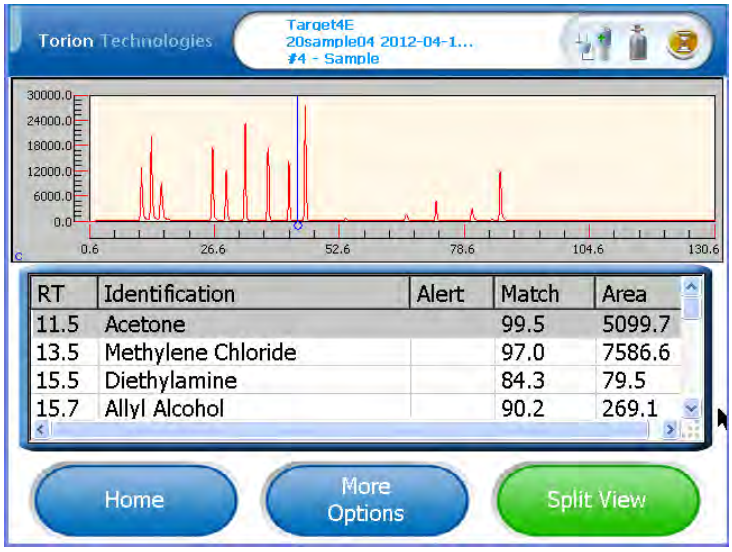


Figure 4-61 Screen displaying end of run data

10. From this final identification screen choose More Options and the following screen will be displayed.

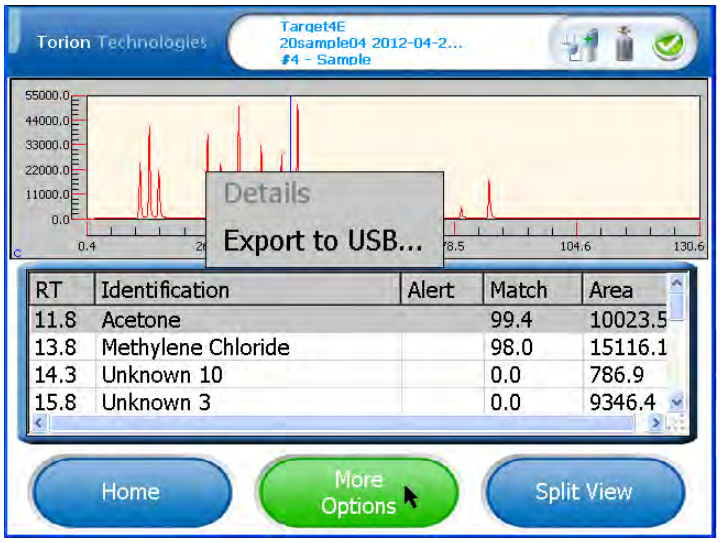


Figure 4-62 Choosing More Options

11. Currently the Details option has not been activated.

12. Choosing the **Export to USB…** button will display the Export files screen as shown above. This functions exactly the same as discussed in the steps above.

Chapter 5

5 Software

This chapter describes how to install and use the various software programs that are included with the instrument.

Software programs

The TRIDION is supplied with several software programs. The following is a list of the various programs and a brief description of what they are used for.

CHROMION™

The CHROMION software is used for instrument control, library management, library-known compound identification interface, multiple instrument control, deconvolution/unknown identification, and creation of methods for use on the instrument. The CHROMION software is also used to view and work with chromatographic and mass spectral data from the TRIDION instrument.

VNC Viewer

This software is used to monitor and control the TRIDION from a PC.

NIST

This is the NIST mass spectral library and software used to interact with the library.

CHROMION Installation and Operation

1. Locate the folder in which the CHROMION *setup.exe* is located.
2. Double-click *setup.exe* to install the program following the instructions on the screen.
3. A CHROMION icon will automatically be installed on the desktop.
4. Double-click on the icon to run CHROMION.

CHROMION Main Screen

1. This image shows the initial screen that appears when opening the CHROMION software.

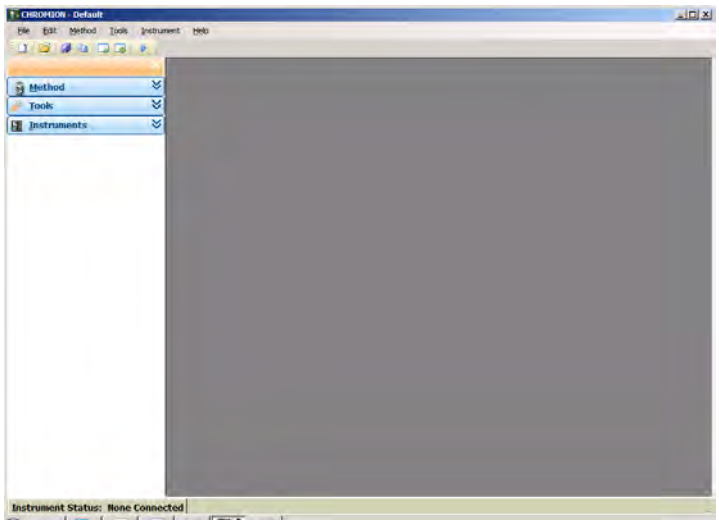


Figure 5-1CHROMION main window

2. There are many ways to navigate within **CHROMION**. The main functions are accessible from the navigation pane on the left side of the screen.

3. In addition to the main functions other functions are available thru the top bar menus, the button bars and by using right click popup menus.

4. The navigation pane on the left side of the screen provides centralized navigation to easily access the **CHROMION** forms which are bundled in different categories such as; **Method**, **Tools** and **Instruments**.

5. When using a lap top it can be useful to hide the navigation pane in order to increase the viewable area of the screen. The **Navigation** pane can be easily hidden and unhidden by clicking on the horizontal expand/collapse arrows located in the orange bar at the top of the pane.

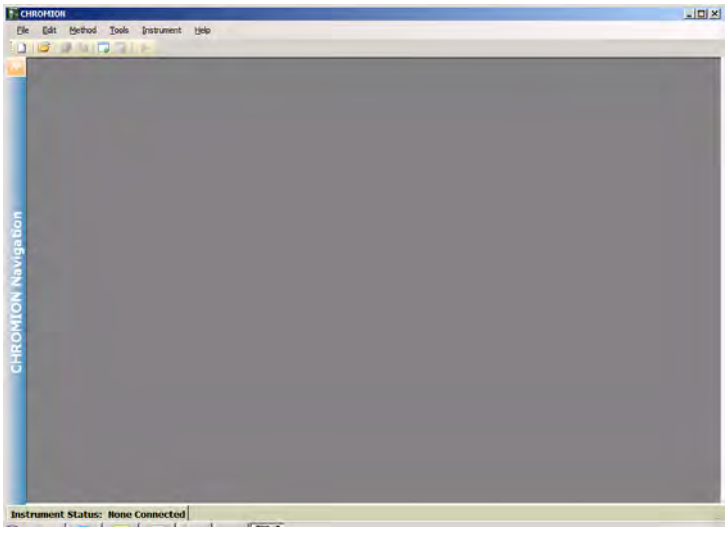


Figure 5-2 CHROMION main window with Navigation pane collapsed

6. Many of the items in the **Navigation** pane open forms that contain specific information used to complete the tasks required to operate the GC-TMS. When a new form is opened additional menu

items and buttons are added to meet the requirements of the open form. The functions of the various menus and buttons will be described later in the chapter.

CHROMION Menu Bar

The following are the menus that are always present on the menu bar. Some of the contents of these menus change as needed for a specific open form.

a. File:
b. Edit:
c. Method:
d. Instrument:
e. Help:

File menu

1. The **Exit** option closes the CHROMION software.

2. When **Data Review** is active an option to open a data file is included in the **File** menu.

3. Data file types currently supported are:

    a. Net.CDF: This is standard mass spectra file type. The header information for this type of file may contain or be missing information that will affect some operations in the **Data Review** part of the software.

    b. *.RAW: This is a Torion file that contains the unfiltered data from the instrument. It can be useful for troubleshooting instrument problems. It is not easy to interpret the data from this type of file. Therefore it is only useful to individuals that have been properly trained.

    c. *.RES: This is a compressed file that contains all of the information used to create a data file on the instrument. The following information is stored in the .RES file:

        i. Net.CDF data File

        ii. *.RAW data file

        iii. Target List information

        iv. Calibration information

            1. Mass

            2. Retention time

        v. Mass spectrometer instrument settings

Edit menu

Preferences...

1. The **Preferences** option opens the following screen. This allows setting of functional preferences for different parts of the software. The functions on will be described in this section of the manual and will only make sense when placed in context of the software section they are connected to. For example the **Data Review** preferences tab is for functions that affect the **Data Review** form. To understand these functions it may be necessary to review the Data Review section of this chapter.

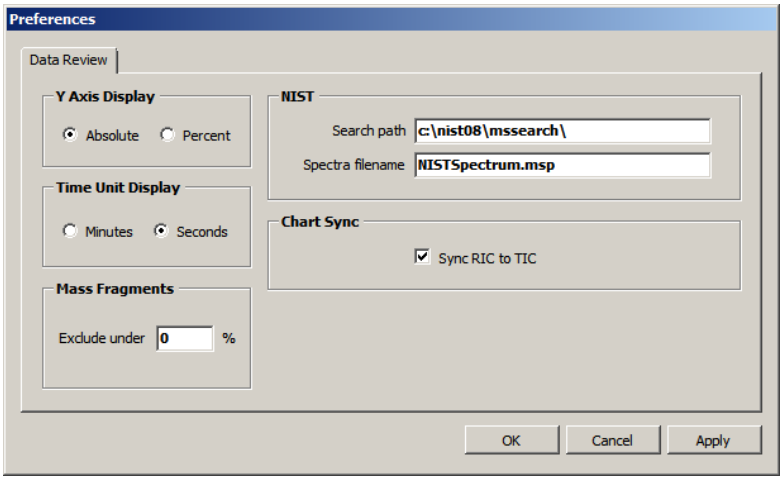


Figure 5-3 Preferences form

2. The **Data Review** tab has settings that affect the **Data Review** form.

    a. The **Y Axis Display** can be set to show the **Absolute** peak intensity of the masses in a given scan or display the relative intensity with the tallest peak set to 100% and the other mass peaks shown as a **Percent** of the tallest mass peak.

    b. The **Time Unit Display** allows the user to set the x axis values to **Minutes** or **Seconds.**

    c. The **Mass Fragments** allows the user to set the display to filter out mass fragments that have a relative percent response below the value set in the **Exclude Under** box.

    d. The **NIST** option allows the user to enter in the path of the NIST software. Type the location of the NIST software into the **Search Path** field. To change the name of the temporary file that is created when exporting spectra to the NIST search, type the desired name in the **Spectra File Name** field.

    e. The **Chart Synch** function ties the x axis values of the TIC and RIC windows to each other. To keep the times synched place a check in the box next to **Sync RIC to TIC**. If you desire to see peaks at different retention times in the RIC and TIC windows leave the box empty.

Hazard Levels...

1. The **Hazard Levels** menu is used to configure safety information that will be displayed on the TRIDION -9 when target compounds have been identified. The following image shows the **Hazard Levels** dialog box.

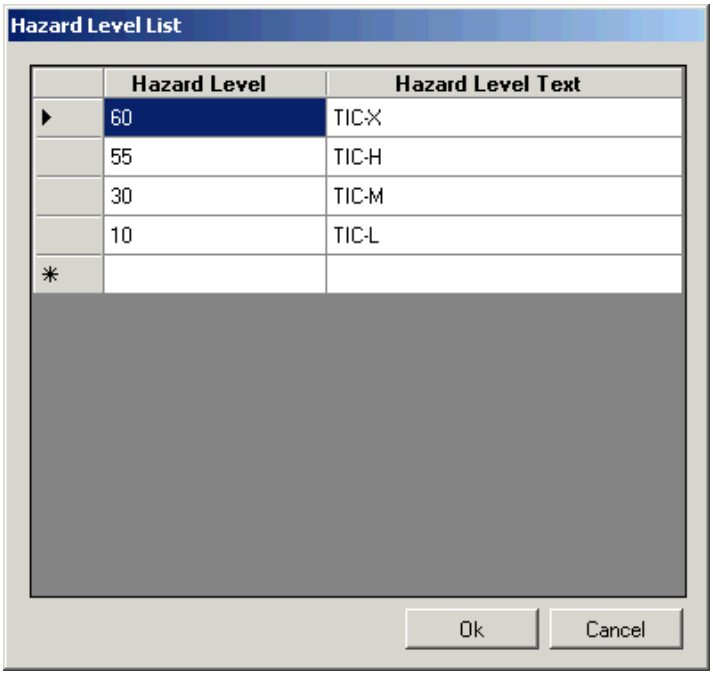


Figure 5-4 Hazard levels dialog box

2. The user can enter any numerical value in the **Hazard Level** column.

3. The user can then enter a text or numeric value in the **Hazard Level Text** column. This allows each user to customize the hazard level information for their specific application.

4. The information that will be displayed on the screen is the information contained in the **Hazard Level Text** column. How to use this information will be described in the **Target List** section of this manual.

5. To remove an entry rick click on the line of the entry and select the remove hazard level entry option.

Instrument Menu

Connecting to an Instrument

1. Before connecting an instrument to CHROMION it must be added to the Instrument List which is located on the **Instrument Setup** form.

2. To add a new instrument to CHROMION click **Instrument** on the main menu and select **Instrument Setup**.

3. Enter an **Instrument Name** the name is just a descriptive label and can be anything that the user enters.

4. Enter the **IP Address** of the instrument being connected and click the **Add** button. To find the address refer to the on instrument software section of this manual.

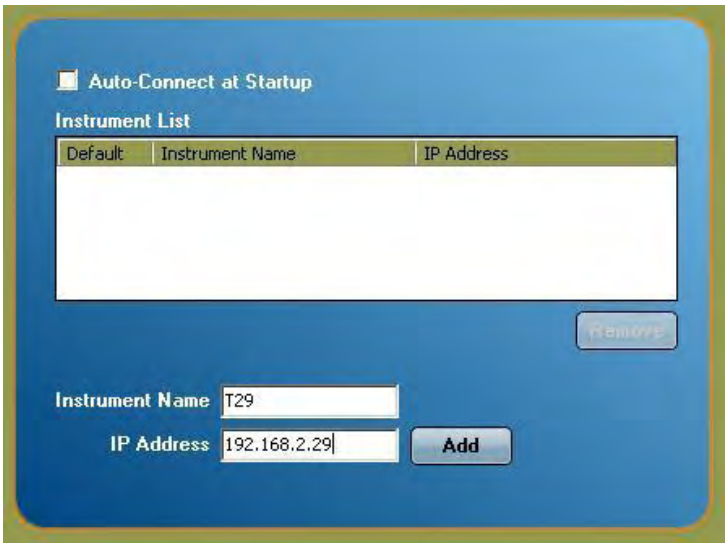


Figure 5-5 Instrument Setup when adding an instrument for the first time

5. Enabling **Auto-Connect at Startup** will reconnect the default instrument each time CHROMION is launched.

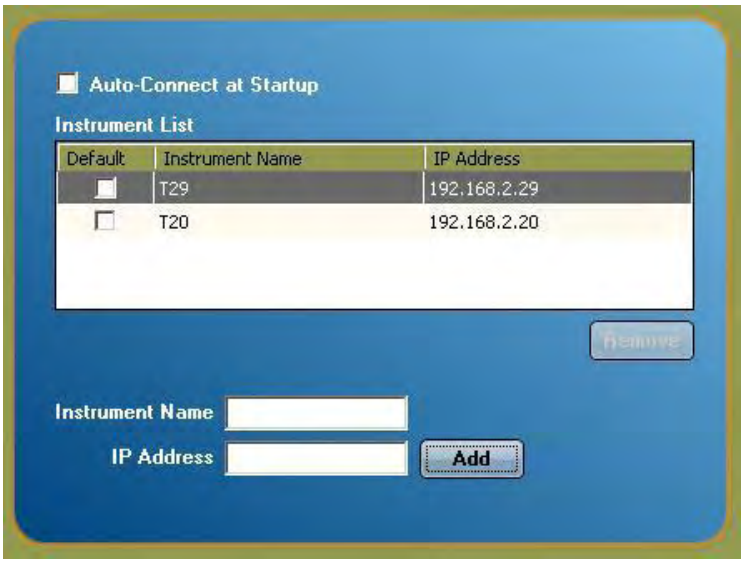


Figure 5-6 Instrument Setup after adding instruments

6. Selecting the check box in the default column will set which instrument is connected when using Auto-Connect at Startup.

7. There are two ways to connect an instrument to CHROMION:

    a. Click **Instrument** on the main menu and choose **Connect Instrument.** Select the **Instrument Name** from the drop-down menu and click **OK.**

Figure 5-7 connect an instrument to CHROMION

b. In the CHROMION navigation pane, click **Instruments** and then click the expand icon for a list of instruments. Right-click and select **Connect to Instrument**.

Note: The taskbar at the bottom of the screen will display the instrument name when the connection is made to the software.

Figure 5-8 Screen showing the icon in the navigation pane has changed to show that instrument T14 is now connected and the instrument name is highlighted in green

8. Only one instrument can be connected to the PC at a time.

9. While it is possible to use many of the software functions when not connected an instrument there are some functions that only work when the computer is connected to an instrument. Details about how the software interacts with connected instruments will be described in the specific sections where this applies.

10. If a connection to an instrument cannot be made an error message will display indicating that CHROMION is unable to connect to the instrument.

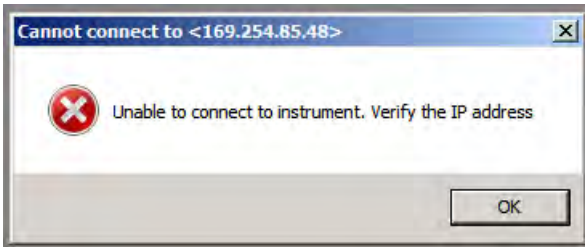


Figure 5-9 Message showing that the software failed to connect to an instrument.

11. In the case where an instrument cannot be connected check the network cables and the IP address settings to ensure they are correct for the type (DHCP server or Direct) of connection you are attempting to make.

Methods Menu

Caution!

The instruments operational parameters for the Gas Chromatograph and Mass Spectrometer can be altered by creating a method in CHROMION and sending it to the instrument. Many of the parameters interact directly with important instrument functions. Be sure to use caution when changing these operational parameters as making inappropriate adjustments will result in poor instrument performance and could cause damage to the instrument.

Method Menu

1. The options available under the **Method** menu are:

   a. **New Method** This opens a dialog box where the user can enter a method name and then creates the method in the database.

   b. **Load/Delete …** This opens a dialog box that allows the user to load a method into the software or to delete methods from the data base.

   c. **Import …** This allows the user to import an exported method. This is a convenient way to move information like target compound lists and GC parameters from one TRIDION-9 to another TRIDION-9.

   d. **Save Method** This saves the method to the data base.

   e. **Save Method As…** This opens a dialog box that allows the user to save the method with a new name.

   f. **Rename Method…** This opens a dialog box that allows the user to change the name of the loaded method.

g. **Export Method** This allows the user to save the method to a file.

h. **Send Method to Instrument** This allows the user to load the method on to the attached instrument. When loading the method there are two choices.

2. All of the menu items are available by clicking on **Method** on the menu bar. The following image shows the **Method** menu.

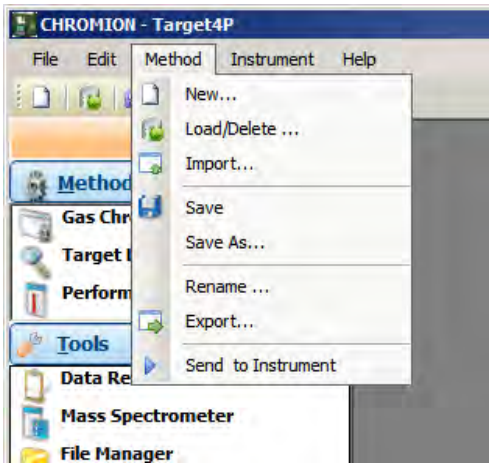


Figure 5-10 Method menu open

Creating a New Method

1. A new method can be created by clicking on **Methods** in the menu bar and selecting **New Method**.

2. When clicking **New Method**the following dialog box will open asking for the user to enter a new method name. By clicking the OK button a new method is created in the database.

Figure 5-11 New Method Name dialog box

3. After creating a new method the method settings forms, **Gas Chromatograph**, **Target List**, and **Performance Validation**, will become enabled under the large **Method** button in the navigation pane.

4. Methods contain a lot of information. In most cases it is easier to open an existing method and under the **Method** menu select **Save Method As** and give the open method a new name. Then edit the method to contain the desired changes.

Load and Delete Methods

1. Selecting the **Load/Delete** option opens the method list. The following image shows the method list.

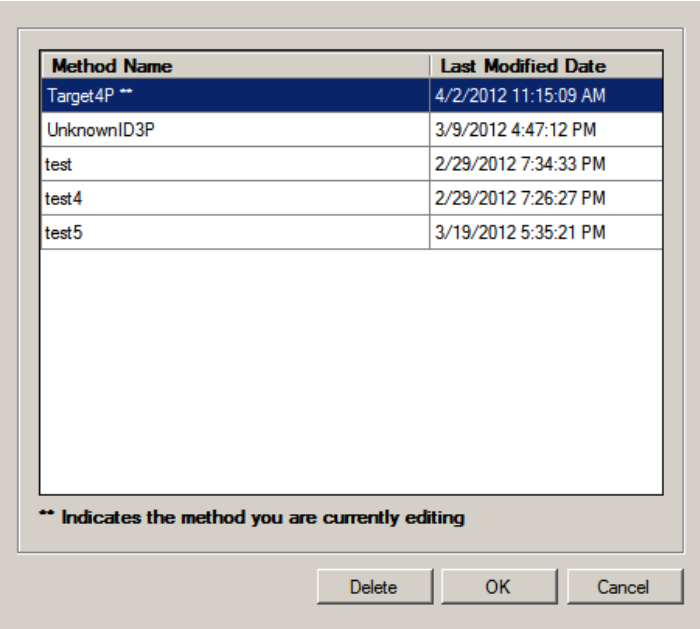


Figure 5-12 Load/Delete Dialog Box

2. Highlight a method by clicking on the name.

3. Select **OK** to load the method.

4. Select **Delete** to delete the method.

Importing a Method

1. The **Import Method** option opens the following dialog box.

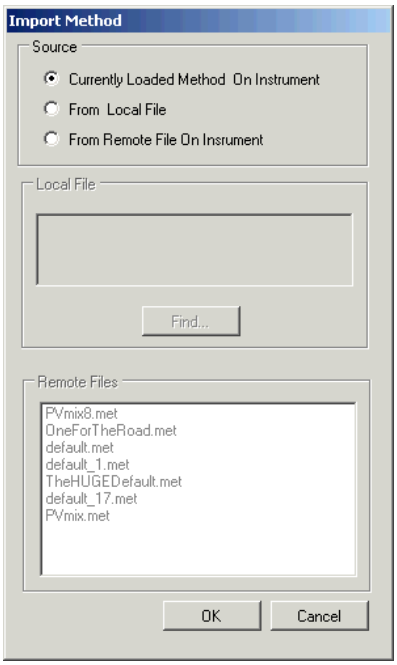


Figure 5-13 Import Method dialog box

2. This dialog box allows the user to import a method into the CHROMION data base from three different locations.

    a. **Currently Loaded Method On Instrument** loads the current method from an attached instrument. If there is no instrument attached this option is not available.

    b. **From Local File** allows the user to navigate to a file location on the PC where an exported method file has been saved.

    c. **From Remote File On Instrument** activates the list of files shown in the **Remote Files** window located at the bottom of the dialog box. The user can open one of the files by selecting it from the list then clicking the OK button. If an instrument is not connected then no files will be visible in the **Remote Files** window.

Saving a Method

1. Select **Save** to save the currently loaded method.

2. The following dialog box will open confirming that the method was saved.

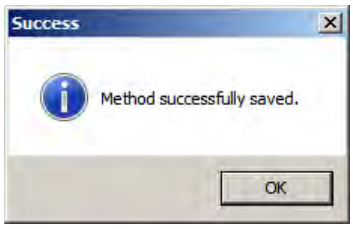


Figure 5-14 Method successfully saved dialog box.

Saving a Method as a New Method

1. Select **Save As…** to create a copy of the currently loaded method with a new name.

2. The following dialog box will open allowing the user to input the method name.

Figure 5-15 Save As... dialog box

4. Type in the name of the new method and select **OK**.

5. Selecting **Cancel** will abort the operation without saving the new method.

Rename a Method

1. The method name can be changed by clicking **Methods** and selecting **Rename Method**. The following dialog box will open.

Figure 5-16 Rename Method dialog box

Exporting a Method to a File

1. When the **Export Method** function is selected the following dialog box is opened.

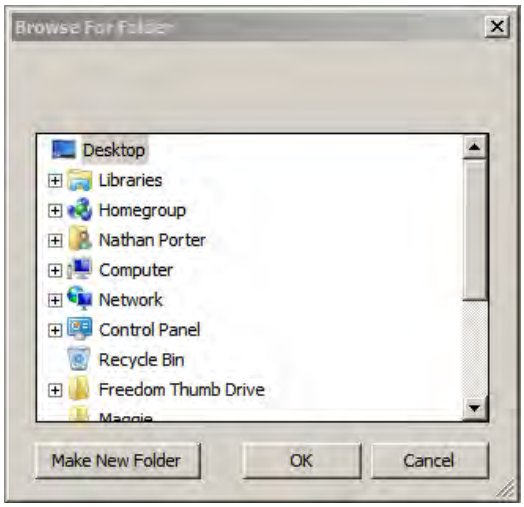


Figure 5-17 Export Method file location dialog box

2. Select the location where the method file will be saved or make a new folder then click OK. The following dialog will open showing that the exported file was successfully created.

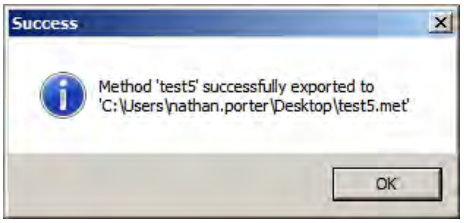


Figure 5-18 Method successfully exported to a file dialog

Send a Method to an Instrument

1. Before sending a method to an instrument it is necessary to save any changes that have been made to the method.

Caution!

Because of the structure of data entry tables in Microsoft Windows™ it is necessary to save a method to ensure that all changes have been accepted. Changing a value in a table and exiting the part of the software where the change was made without first saving the change can result in the value reverting back to the original value.

2. Selecting **Send Method to Instrument** send the loaded method to the currently connected instrument.

3. The following dialog opens.

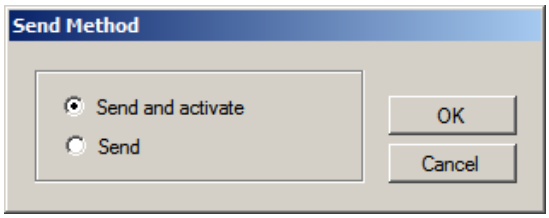


Figure 5-19 Send Method dialog box

4. The user has two options:

    a. **Send and activate** sends the current method to the connected instrument and makes the method the active method.

    b. **Send** sends the current method to the connected instruments SD card for later use.

5. The following dialog box opens to confirm that the method was successfully sent.

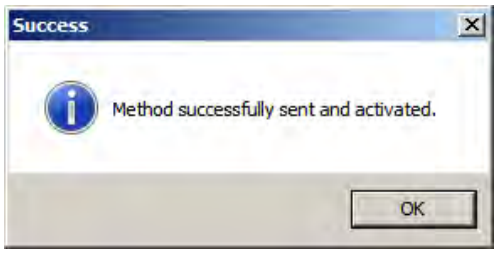


Figure 5-20 Method successfully sent and activated dialog box

6. If the **Send** option was selected the dialog box will indicate that the method was sent but will not say that it was activated.

7. If the send fails a dialog box will open that indicates that the method did not reach the instrument. If this happens try resending the method. If the failed to send message continues to appear restart the instrument and reestablish communication. If the fill cannot be sent contact Torion for assistance.

8. If there is no instrument connected the following dialog box will appear. If this happens check your instrument connections.

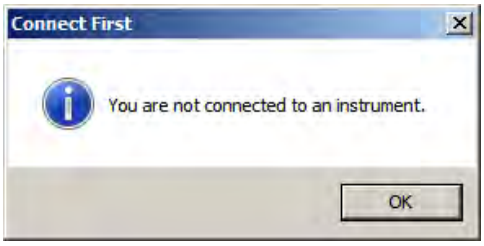


Figure 5-21 You are not connected to an instrument dialog box

9. All of the functions of the **Method** menu are also available on the button bar that is located above the expanded navigation menu on the left side of the screen. The following shows the button bar with the text for each of the buttons.

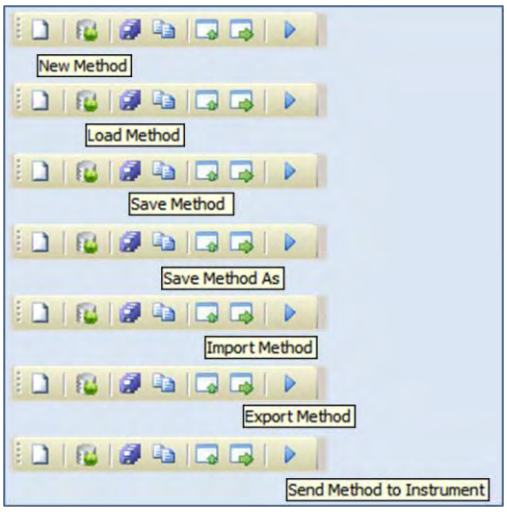


Figure 5-22 Method Button Bar

10. Clicking on a button activates the exact same activity at those described above.

Gas Chromatograph

Gas Chromatograph Buttons

1. The following shows an image of the Gas Chromatograph buttons with pop up descriptions.

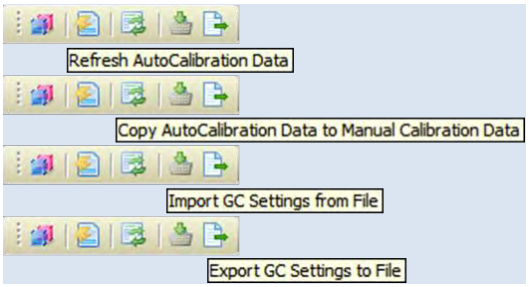


Figure 5-23 Gas Chromatograph button bar with descriptions

2. **Refresh AutoCalibration Data:** Clicking this button reads the auto calibration information for the retention times from an attached instrument. It is used when the user suspects that the retention information has changed on an instrument after a method was last used and the user wants the method to reflect the changes.

3. **Copy AutoCalibration Data to Manual Calibration Data:** This function allows the user to run an auto calibration run then if they want to make changes manually they can copy the auto calibration data to the manual calibration table and modify the information. This button is only available in the **Retention Time Calibrations** tab.

4. **Import GC Settings from File:** This allows the user to import GC settings that have been exported from another method. This button is only available in the **Retention Time Calibrations** tab.

5. **Export GC Settings to File:** This allows the user to export GC settings to a file so they can be imported into another method file.

GC Parameters tab

1. When an instrument is attached the settings for Gas Chromatograph are displayed as in the screen below.

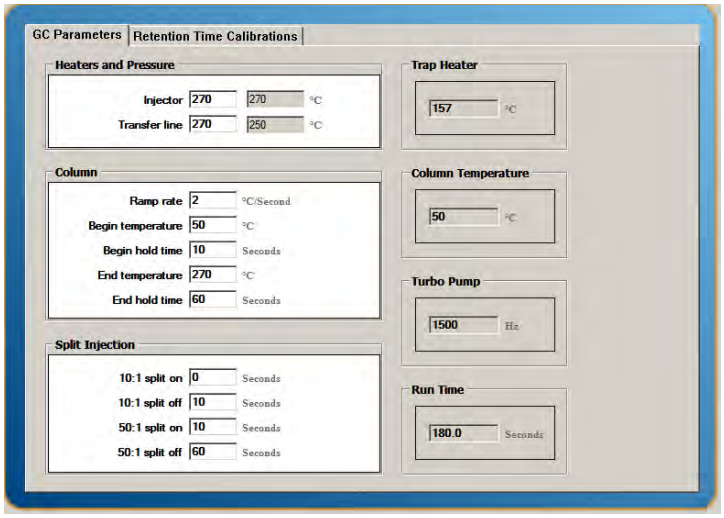


Figure 5-24 Gas Chromatograph control

2. The **Heaters** section displays the set points for the gas chromatograph.

    a. **Injector:** The temperature is normally set to 270°C. The maximum temperature is 300°C.

    b. **Transfer Line:** The temperature is normally set to 270°C. The maximum temperature is 270°C.

3. The **Split Injection** section is used for controlling the GC inlet's split injection controls. Normal operation is to run with the split values open. To introduce more sample into the GC column the valves should both be closed for 1 to 2 seconds. To do this the user would set the **Split On** time to 2 seconds, telling the instrument to turn the split on at 2 seconds, this will keep the valve closed after the sample is injected for 2 seconds then it will open to sweep the injector. Turning the split on for longer times will have a detrimental effect on the peak shape of early eluting peaks. Later eluting peaks will refocus at the head of the column so they will not be as adversely affected.

    a. The **10:1 Split On** opens the lower flow split valve at the time the user defines. Normal setting is to turn on the split at time 0.

    b. The **10:1 Split Off** closes the lower flow split valve at the time the user defines. Normal setting is to turn off the split at 10 seconds.

    c. The **50:1 Split On** opens the higher flow split valve at the time the user defines. Normal setting is to turn off the split at 10 seconds.

    d. The **50:1 Split Off** closes the higher flow split valve at the time the user defines. Normal is to turnoff the split at 30 seconds.

Retention Time Calibrations tab

1. The Retention Time Calibration tab is used to set up the instrument to determine retention index values.

2. Using retention index times makes it easier to transfer methods between instruments. In addition, using retention indexes allows the user to modify the GC method without losing peak identification information.

3. The target list uses retention times to narrow the library search. If the gas chromatographic method is changed then the retention times will also change. The change in retention times will invalidate the target list since the compounds will have retention times that are different than that setup in the target list.

4. Retention indexes were developed to make it possible to compare data from a variety of instruments using similar columns but different oven programs. One of the most common indexes is the Kovats index. All straight chain hydrocarbon molecules are assigned an index value of 100 per carbon. So a molecule like heptane with 7 carbons would have a Kovats value of 700. And a molecule like tetradecane with 14 carbons would have an index value of 1400. The retention time calibration uses the following compounds that are included in the CALION standard vial.

Compound	Retention Index
Methylene Chloride	531
Toluene-d8	759
Bromoform	853
Tetradecane	1400

5. If retention indexes are used in the target list then simply calibrating the retention time allows the same target list to work on another instrument or with different gas chromatography ramp rates or hold times.

6. The user does need to adjust the retention time windows used in the performance validation to reflect the new times that result from differences between instruments or the changed GC parameters.

7. This section includes the following functions:

8. **Manual Calibration Data** allows the user to enter values in the calibration table. This allows the user to enter a retention index value for a specified retention time.

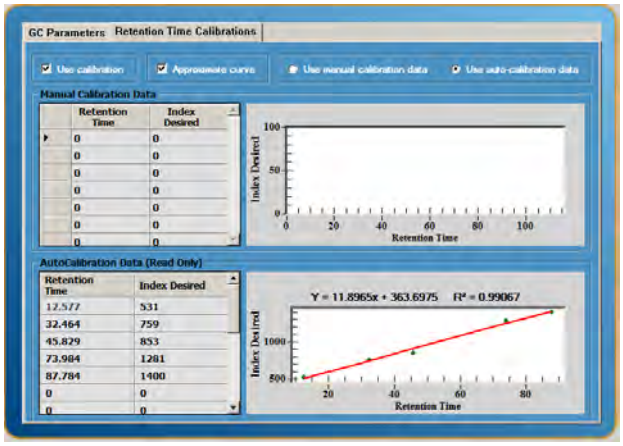


Figure 5-25 Gas Chromatograph Retention Time Calibration

9. **Auto-Generated Calibration Data** uses the auto-calibration function to automatically create retention index values from the performance validation data. How to enter data into and verify the correctness of the performance validation table will be discussed in the next section.

10. **Use manual calibration data or Use auto-calibration data:** selects which table of data to use to create retention index values for the peaks in a sample run.

11. **Use calibration** sets the method to either use the retention index or not.

12. The **Approximate curve** option allows the user to select to use a single linear calibration for the retention index curve. If **Approximate Curve** option is unchecked then the system uses a point to point piece wise fit.

Target List

Target List Buttons

1. The following image shows the buttons that attached to the Target List screen.

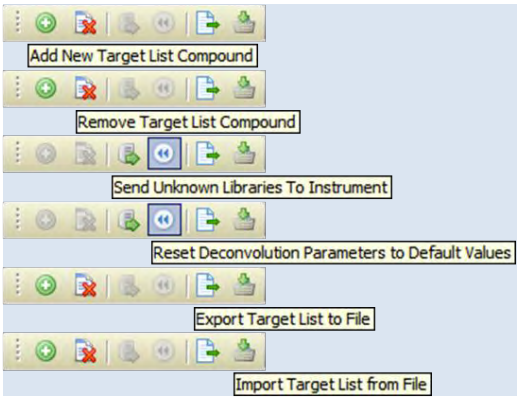


Figure 5-26 Target List buttons with captions

2. **Add New Target List Compound:** Clicking this button inserts a line at the end of the compounds list. Details about how to enter a new compound are described below. This button is only available in the **Target List** tab.

3. **Remove Target List Compound:** Clicking this button will remove a selected compound from the target list: Details about how to remove a compound from the target list is described below. This button is only available in the **Target List** tab.

4. **Send Unknown Libraries To Instrument:** If a library has been referenced on the **Deconvolution Parameters** tab then the user can send the referenced library to the instrument. Depending on the size of the file sending files to the instrument can take from a few seconds to a few minutes. Because of the potential size of the library files the libraries are not sent every time a method is sent. This button is only available in the **Deconvolution Parameters** tab.

5. **Reset Deconvolution Parameters to Default Values:** Clicking this button resets the **Deconvolution Parameters** to factory defaults. All changes to the parameters will be lost. This button is only available in the **Deconvolution Parameters** tab.

6. **Export Target List to File:** This opens the normal Windows file save dialog box and allows the user to save the Target List as a file for use in other methods.

7. **Import Target List from File:** This opens the normal Windows open file dialog box and allows the user to open a previously exported Target List.

> **Note**
>
> Importing and exporting **Target Lists** can result in poor compound identification since the retention times for a different method or different instrument may not be consistent with the times used in the **Target List**.

Target List Tab

1. The target list is a subset library used to target compounds of particular interest to the user. It is different from the unknown library because it contains specific information that is influenced by some of the instrument settings.

2. In addition to mass information the target list also contains retention time information. The same list of compounds will be used for configuring quantitative information.

3. The **Masses** table shows the specific ions that are associated with a compound in the target list. The following image shows the masses for 1,1 Dichloroethene.

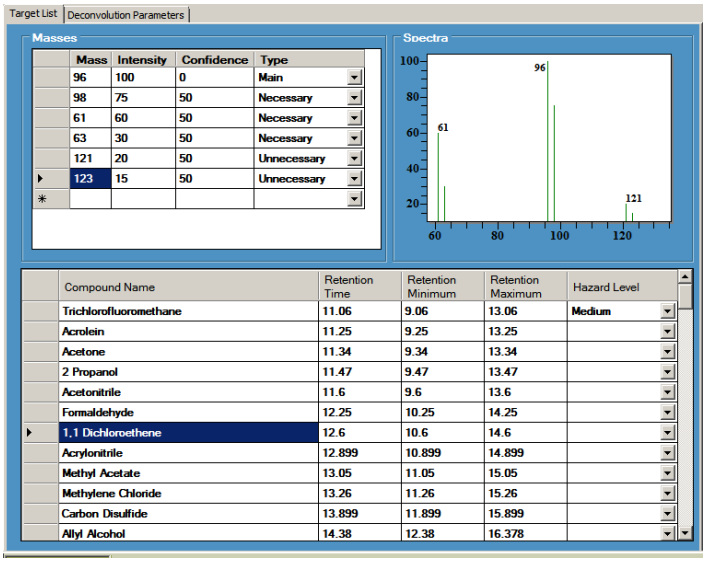


Figure 5-27 Target List

4. Normally the tallest mass peak is designated as the **Main** ion and has an **Intensity** of 100. Each of the other masses has an **Intensity** that is some percentage of the parent peak. For example the 98 mass has an expected intensity that is 75% of the parent peak. The **Confidence** is an absolute value. So the **Confidence** level for the 98 mass is 50. This allows the 98 mass to vary from 25% of the parent peak to 125% of the parent peak and still be acceptable.

5. There are three options for the **Type** column. They are **Main**, **Necessary** and **Unnecessary**.

6. As described above there is only one **Main** mass peak and it is usually the largest peak in the spectrum. It is always assigned the value of 100%.

7. All other masses can be defined as being **Necessary** or **Unnecessary**. **Necessary** masses must be present in a spectrum or the search algorithm will not identify the peak. **Unnecessary** masses are in the spectrum but are not used by the search algorithm to identify a compound. **Unnecessary** masses are usually masses that are less than 20% of the main mass.

8. The values in the masses table can be edited by highlighting the entry with the mouse and typing in the new value.

9. Clicking the right mouse button on a mass opens the delete mass option. If a mass is deleted by accident exit the program without saving the method, when prompted to save the method select no. Then reopen the software and the method will be the same as before the mass was accidentally deleted. Once a method has been saved there is no way to undo any previous actions. It is always wise to keep a backup of important methods so the user can easily return to a n earlier unchanged version of the method.

10. The **Spectra** window shows graphically the information that is in the **Masses** table.

11. The main table is the actual **Target List**.

12. The **Compound Name** column is where the name of a target compound is entered. This column can accept any typed in name.

13. The **Retention Time** column shows the retention time for a compound.

14. The **Retention Minimum** and **Retention Maximum** set the window for the compound identification.

15. The **Hazard Level** is a self configured value. The information displayed in the **Hazard Level** column can be configured by selecting the **Edit** menu at the top of the screen and selecting the **Hazard Level** option. Information about entering information into a **Hazard Level** table is given in the menu section under **Edit/Hazard Level**.

16. To select a **Hazard Level** Click the drop down arrow and select the desired Hazard Level from the list.

17. Since this data is created by the user it can be setup to display any information desired. For example it can be used simply as present or not present option for applications where the chemicals being analyzed are not considered hazardous.

Deconvolution Parameters Tab

Target List Search

1. There only a few items in the **Deconvolution Parameters** that should be adjusted. The following image shows the **Deconvolution Parameters** screen.

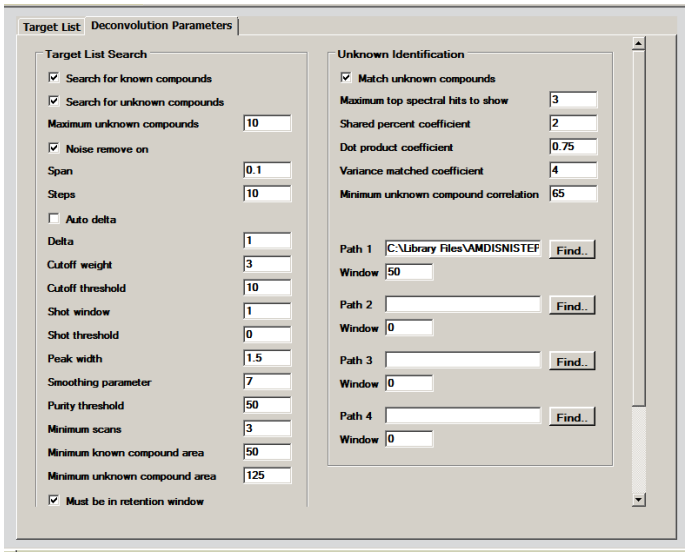


Figure 5-28 Deconvolution Parameters screen

2. The **Search for known compounds** check box enables the deconvolution algorithm to extract the spectra of target compounds and compare the extracted spectra to the **Target List**. The default is for this to be checked. Unchecking this option will result in the search algorithms not returning matches for compounds it the **Target List**.

3. The **Search for unknown compounds** check box enables the deconvolution algorithm to extract and save the spectra of compounds that are not found in the **Target List**. It does not search the unknown library it only allows for the extraction of the spectra.

4. The **Maximum top spectral hits to show** allow the user to specify the number of unknown compounds to display in either the CHROMION software or on the instrument. If a chromatogram has a large number of small peaks allowing deconvolution and display of all of them will result in slowing down the on instrument post run data processing. The default of 10 is a good compromise that allows for significant peaks to be identified while limiting the burden on the instrument processor.

5. The Noise Remove check box turns on and off the noise removal portion of the deconvolution algorithm. Unchecking this box will result in poor spectral extraction and potential miss identification of compounds.

6. All of the remaining settings are used to adjust the deconvolution and baseline extraction routine. The current settings are optimized to provide optimum performance for deconvolution and should not be changed. Changing these setting will affect the deconvolution process. They should only be changed by personnel that have been trained in their function. Contact the Torion for more information.

Unknown Identification

1. The **Match unknown compounds** check box turns on and off the library search for unknown compounds that are not part of the **Target List**.

2. The **Maximum top spectral hits to show** set the number of compounds that will be displayed with the compounds shown in order of quality of fit.

3. All of the remaining settings are used to adjust the unknown search routine. The current settings are optimized to provide optimum performance for identifying unknown peaks. Changing these setting will affect the identification process. They should only be changed by personnel that have been trained in their function. Contact the Torion for more information.

4. The **Path 1, Path 2, Path 3 and Path4** allow the user to designate the location of unknown libraries to search. The search will be conducted by looking in the first path then in each successive path until the best match is found. These libraries will be stored on the SD card on the instrument and should be limited in the number of compounds to keep the data processing time reasonable.

5. The **Window** refers to retention index window to be used. Part of the search algorithm uses retention index. The window is normally set to 75.

Performance Validation

1. The **Performance Validation** is used to setup the information used for calibration of both retention time and mass. The following image shows the performance validation screen.

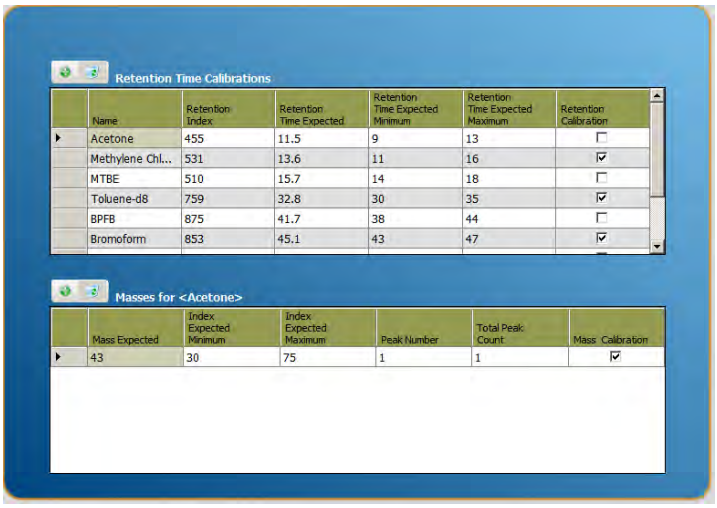


Figure 5-29 Performance Validation window

2. The following is a description of each of the columns in the **Retention Time Calibrations** table.

   a. **Name:** This column is used for the names of the standards that will be used for the calibration and validation of the instrument performance.

   b. **Retention Index:** These are retention index values from the NIST data base. A description of retention indexes and how they are used is provided in the **Retention Time Calibration** section of this manual.

   c. **Retention Time Expected:** This is the time that the compound is expected to elute from the instrument. If the **Gas Chromatography** method is changed then it is necessary to run the standard mix and adjust the retention times in the **Performance Validation** table.

   d. **Retention Time Expected Minimum** and **Retention Time Expected Maximum:** are used to set a window of time where the automatic calibration routines would expect the compound listed in the table to elute.

e. **Retention Calibration:** If the compound is to be used by the auto calibration routine to calculate the retention indexes of unknown compounds. The compounds where the box is left unchecked are used for mass calibration not retention time calibration.

3. Above the **Retention Time Calibrations** table are two buttons

4. The first button is used to add compounds to the table. To add compounds highlight a position in the table and click the **Add Compound** button. A new line will appear at the bottom of the table. Type in the name of the compound and fill in the numeric values for the other columns.

5. If a value is entered that is not acceptable a red exclamation point will be shown in the column on the far left. The following image shows an error in the last column of the table next to Ethyl Acetate. In this case a letter has been entered into a numeric value only field (**Retention Index**). If this happens the software will not allow the user to change to another field until the error situation has been corrected.

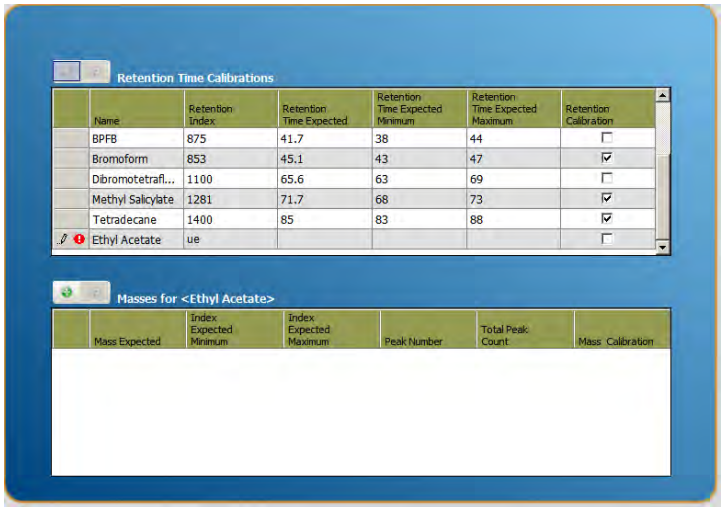


Figure 5-30 Performance Validation screen showing an error in data entry

6. To remove a compound use the mouse to highlight the compound in the table then click the **Remove Compound** button which is the second button from the left with the trash can on it. The following image shows the dialog box that opens after clicking on the **Remove Compound** button.

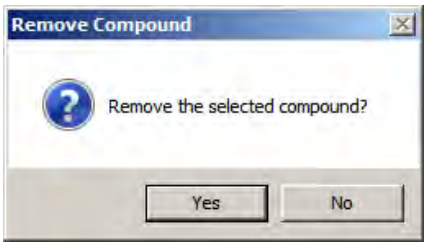


Figure 5-31 Performance Validation Remove Compound dialog box

7. Selecting yes will remove the compound from the table.

8. The **Masses for <compound name>** table displays the selected masses for a specific compound.

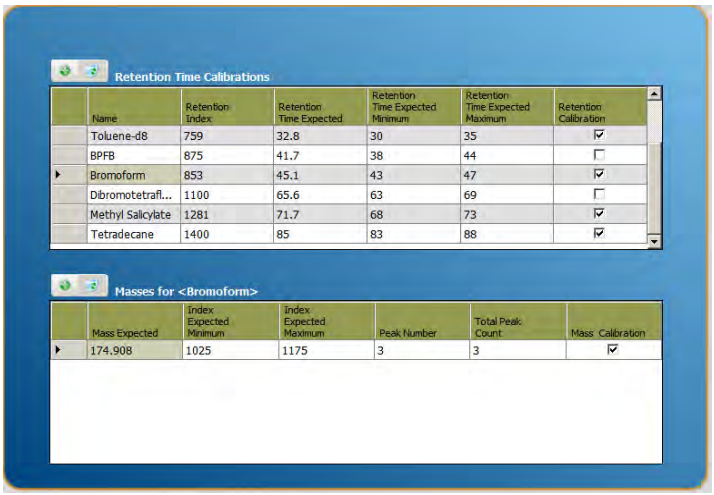


Figure 5-32 Performance Validation showing Masses for Bromoform

9. The TRIDION-9 instrument has approximately 4000 bins for mass data. Each mass has a width of about 8 bins. To convert the index numbers to actual mass values it is necessary to assign a specified mass to a specific index number. The auto calibration routine built into the instrument will apply the calibration automatically. The mass information is stored in the **Mass for <compound name>** table. The data that are entered into the table are described below.

10. The following are the columns for the **Masses for <compound name>** table.

    a. **Mass Expected:** This column is where the mass to be used for calibration that is in a specific compound is entered here. In the above example the 174 mass found in bromoform has been entered.

    b. **Index Expected Minimum:** In the above example this is the lowest index (bin) number that the user would expect the 174 mass to elute.

    c. **Index Expected Maximum:** In the above example this value is the highest index (bin) number that the user would expect the 174 mass to elute.

    d. **Peak Number:** To improve the accuracy of the calibration the user can specify a peak number. For example bromoform has a group of masses at 170, 172, and 174. Since the last peak in a group is less susceptible to trap overloading effects we would choose to use mass 174 for calibration. In this case mass 174 is peak number 3 of the group so we would enter a value of 3 for the peak number.

    e. **Total Peak Count:** Total peak count specifies the number of mass peaks expected in a group of peaks. In the case of bromoform there are three peaks to the **Total Peak Count** would be 3.

    f. **Mass Calibration:** Placing a check box in this column sets the auto calibration routine to use the specified mass. Leaving the box unchecked allows the user to leave the information in the table but not use it for the calibration.

11. Above the **Mass for <compound name>** table are two buttons

12. The first button is used to add masses to the table. To add calibration masses highlight a position in the table and click the **Add calibration Mass** button. A new line will appear at the bottom of the table. Type in the numeric values in the columns.

13. If a value is entered that is not acceptable a red exclamation point will be shown in the column on the far left. The following image shows an error in the last column of the table next to 172.809. In this case a letter has been entered into a numeric value only field (**Index Expected Minimum**). If this happens the software will not allow the user to change to another field until the error situation has been corrected.

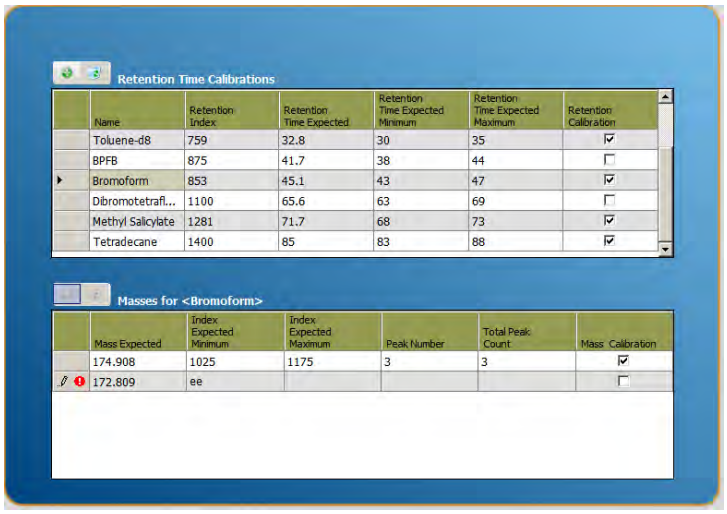


Figure 5-33 Performance Validation screen showing an error in data entry

14. To remove a mass use the mouse to highlight the mass in the table then click the **Remove Calibration Mass** button which is the second button from the left with the trash can on it. The following image shows the dialog box that opens after clicking on the **Remove Calibration Mass** button.

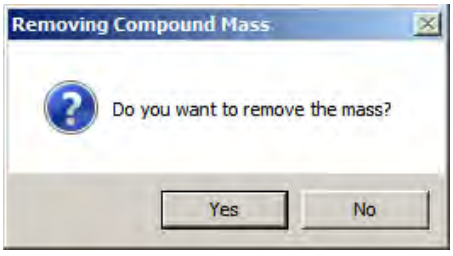


Figure 5-34 Performance Validation Removing Compound Mass dialog box

15. Selecting yes will remove the mass from the table.

Tools

1. The Tools section of the navigation pane contains functions that are not part of a method. Method components affect things like retention time generation and actions that rely on retention times, like target compound identification and calibration. These are primarily gas chromatographic functions

2. The functions in the tools section are either generic and not specific in nature or very specific for a single instrument.

Overview of Data Review

1. Below is an image of the Data Review form. The following are descriptions of the different file types that can be reviewed by Data Review:

a. .RES is a results file. This file contains all of the information that is used to create a set of data. This includes the data in both the CDF format and the RAW format. These are explained below. The results file also contains the target library and search results. A report file in the form of a text file is included. The report has the same information as the report on the TRIDION-9 instrument. In addition, the results file also contains the setting.xml file that contains the mass spectrometer and GC parameters and the .ini file for the tuning wizard. It is recommended that the user work with the results files since all of the information needed to repeat an experiment is contained in this file. Just using the CDF and/or RAW data files does not provide enough information to later recreate the method and settings used to get the data.

b. .CDF is a **C**ommon **D**ata **F**ormat file type used for chromatographic and mass spectral data. It contains all of the information needed to display the chromatogram and mass spectra in the correct format for peak identification.

c. .RAW is a format of data that is produced directly by the instrument. The mass spectral data has not been calibrated and does not display masses, rather is displays indices. It is not sorted and labeled so that it can be used to compare to traditional data. In addition, it has not been processed using the auto-ionization algorithms. It is used for diagnostic purposes to determine the performance of an instrument.

d. .CSV is a standard file type that can be opened in most spreadsheet programs like Windows Excel. These files are created by the user through export functions.

2. Data can be directly opened from a .RES, .CDF or .RAW file. In the case of the .RES file the users can choose between opening the CDF file or the RAW file. The following image shows the open file dialog with the file type drop down menu visible.

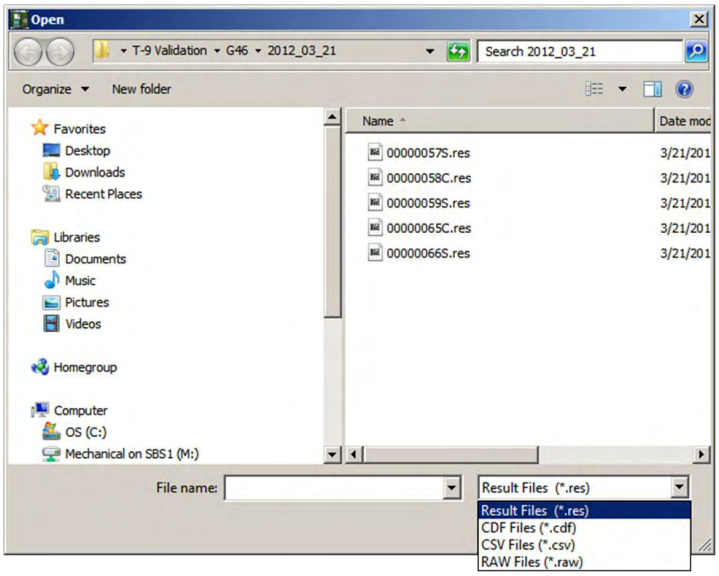


Figure 5-35 Data Review open file dialog box showing file types

3. The following image shows the dialog box that opens when the user opens a .RES type of file.

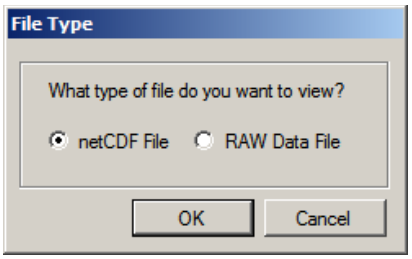


Figure 5-36 File Type option box that is displayed when opening a file with the .RES extension

4. Selecting the **netCDF File** option will open the CDF file that is in the results file. Choosing the **RAW Data File** will open the raw data that is in the results file.

5. The following image shows a CDF data file open in the data review window.

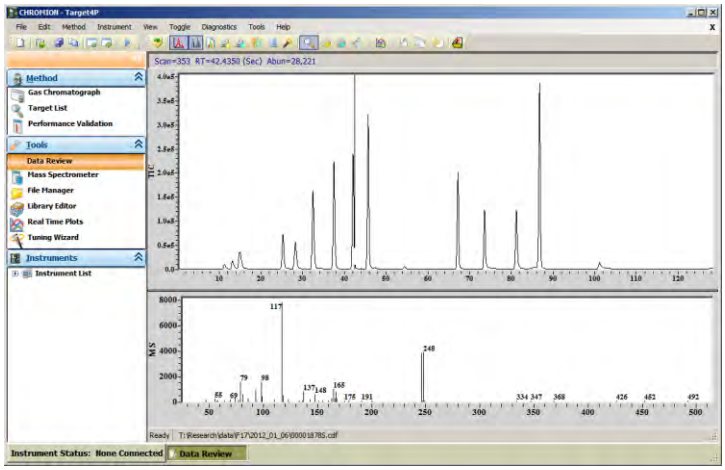


Figure 5-37 Data Review window with a CDF file open

6. **Print Chart:** From the popup menu in any graph the user can print the chart. The print option uses the windows default printer to print the chart. To change to a different printer go to control panel in the Windows operating system and open devices and printers and change the default printer to the printer you want used.

Data Review Button Bar

1. The button bar specific to the **Data Review** part of the software is located directly above the data window.

2. The following image shows the button used for opening a data file. The open file dialog box can also be opened using the files menu.

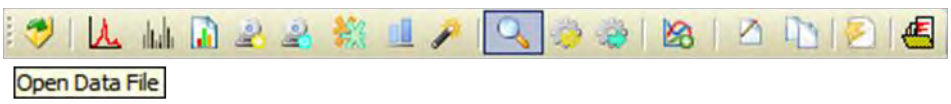


Figure 5-38 Data Review Button bar showing the location of the open file button

3. The following image shows the Data Review button bar with labels for the buttons that are used to show graphs.

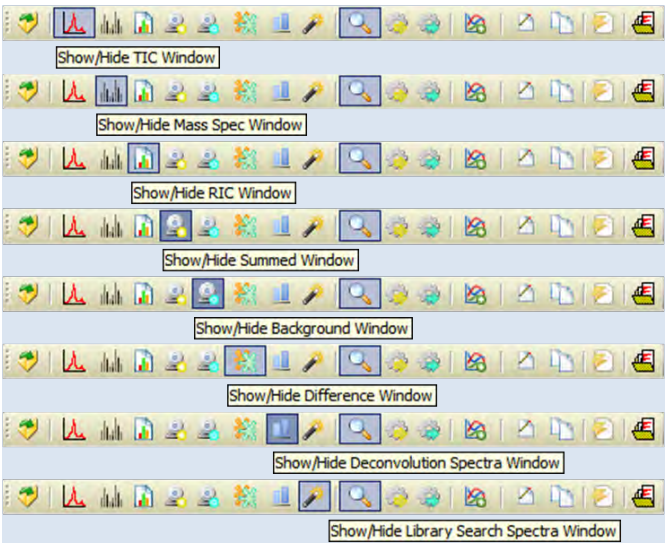


Figure 5-39 Data Review button bar with labels for the buttons that are used to show graphs

4. All of these functions are also available through the menus in the software.

5. The following are descriptions of the graphs that are opened by the buttons.

    a. **TIC**: Total Ion Chromatogram. This is the GC trace of the entire signal that is generated by the mass spectrometer. The following Image shows the TIC graph window open with no other graphs being displayed.

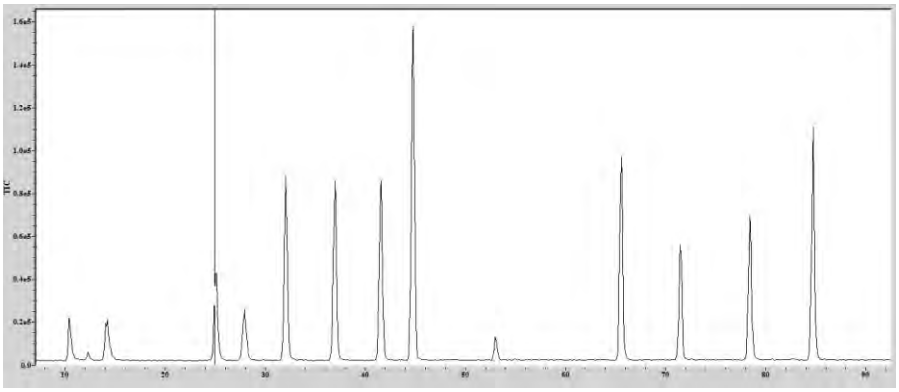


Figure 5-40 TIC graph showing TIC of 13 compound calibration standard

    b. **MS:** Mass Spectra. This is the spectra for a single scan in the TIC. The spectra displayed are selected by the placement of the cursor. The following image shows the MS graph open with the TIC. The spectrum that is shown is for the scan where the cursor is positioned in the TIC graph.

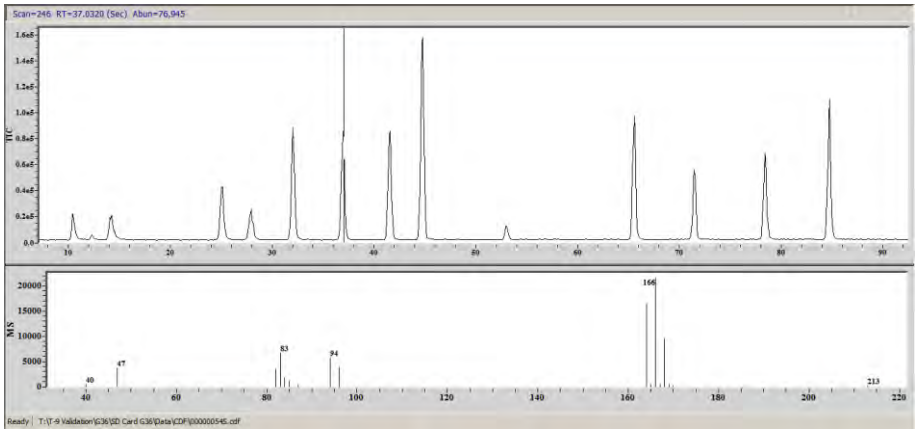


Figure 5-41TIC and MS graphs

c. **RIC:** Reconstructed Ion Chromatogram. This is the chromatographic trace for selected masses and can be used to look for a specific peak with a given mass or group of masses. The following Image shows a RIC graph with a TIC and MS graph open.

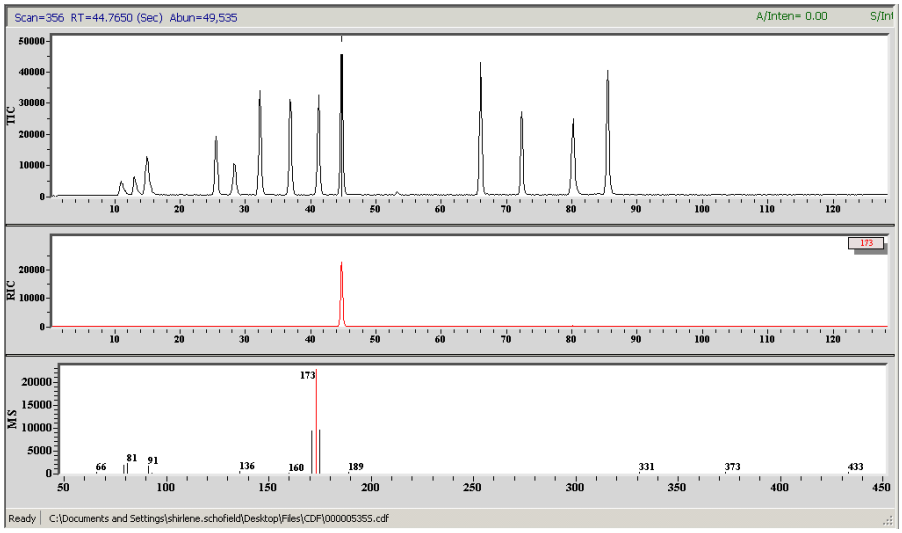


Figure 5-42 RIC graph with TIC graph and MS graphs

d. **Summed:** This is the spectra of a group of chromatographic scans that have been selected using the **Summed** function. Choosing this function totals the response of all of the ions in the region that has been selected. The following image shows a selected area in the TIC for summing (yellow highlight). With the MS graph and the Summed graph showing that the intensity of the ions in the summed graph is much higher than the intensity of the ions in the MS graph.

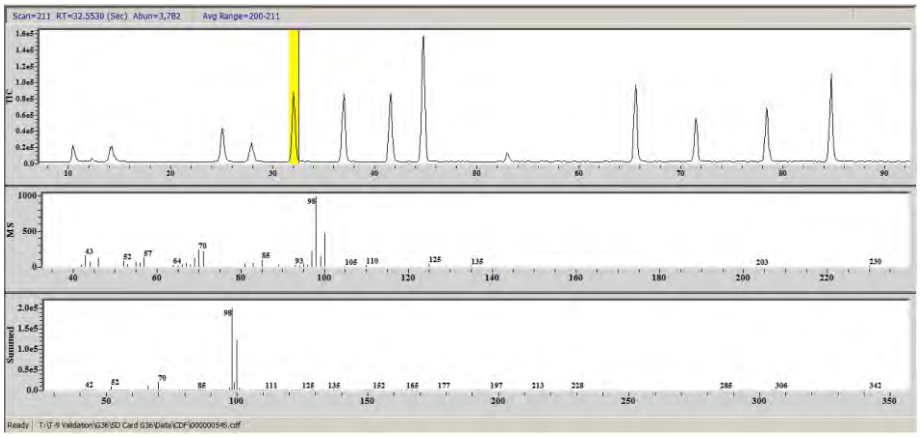


Figure 5-43 Summed graph with TIC and MS graphs

e. **Background:** This is the spectral data for a section of background selected by the user. Choosing this function totals the response of all of the ions in the region that has been selected. The following image shows background (blue) and summed (yellow) areas selected in the TIC graph. The background graph (**Bknd**) shows the background noise of the instrument.

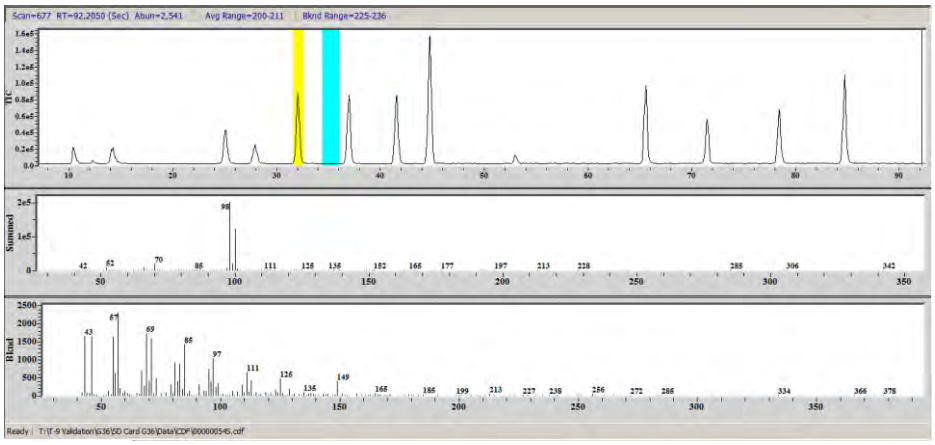


Figure 5-44 Background (Bknd) graph with TIC and Summed graphs

f. **Difference:** This is the spectral data showing the difference between the background spectra and the highlighted section of summed spectra. The following image shows the **TIC** with summed (yellow) and background (blue) areas highlighted and with the difference graph shown (**Diff**). The difference graph shows the background subtracted from the summed values.

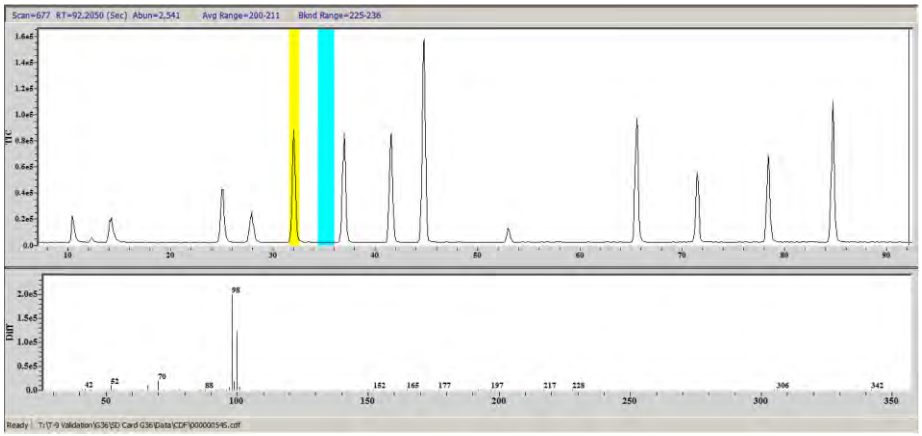


Figure 5-45 Difference (Diff) graph with TIC graph

g. **Deconvolution Spectra**: This shows a graph of the spectra for a single scan in a deconvolved TIC. More detail about how to use this feature will be provided in the discussion about the deconvolution control window later in this manual. The following image shows the deconvolution graph with the TIC graph. The deconvolved peaks are shown in different colors and can be shown in the deconvolution graph by clicking on the peak in the TIC. The toluene-d8 peak has been highlighted and the purple is bolded. The purple spectra are seen in the deconvolution graph.

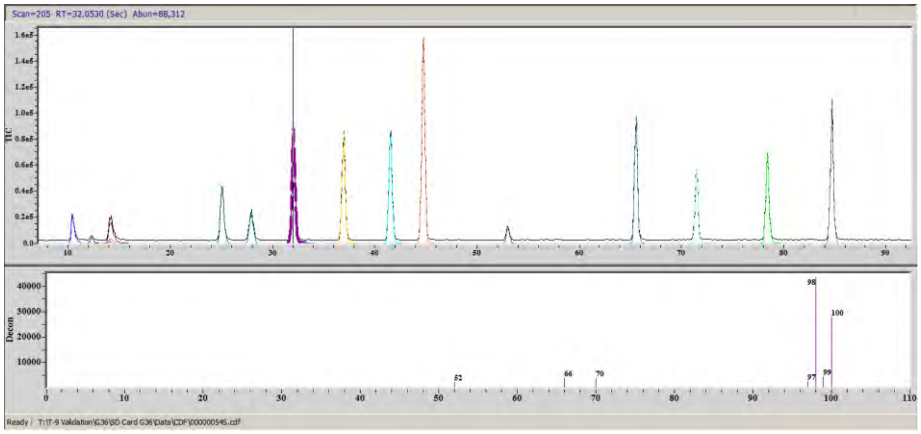


Figure 5-46 Deconvolution (Decon) graph with TIC graph

h. **Library Search Spectra**: This shows head to tail spectra comparing the library spectra to the sample spectra. The following image shows the library spectra compared to the instrument spectra.

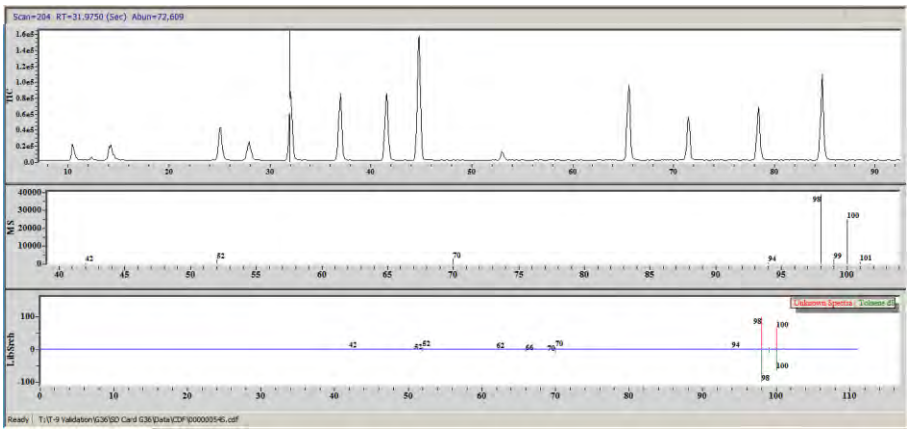


Figure 5-47 Library Search Spectra (LibSrch) graph with the TIC and MS graphs

6. The next three buttons are used to set the cursor mode. The following image shows these buttons highlighted with their labels.

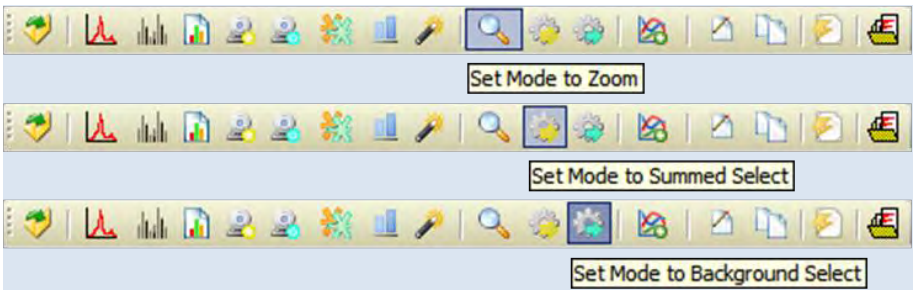


Figure 5-48 Data Review button bar with cursor mode buttons highlighted and labeled

7. The following describes the different cursor modes.

   a. **ZOOM:** When the cursor is set to the zoom mode the user can enlarge parts of any of the graphs that are open. To zoom in the user uses the mouse to drag a box around the area they want to zoom in on. To activate Unzoom move the mouse so the pointer is over the graph that is being worked on. For example to unzoom the TIC use the mouse to place the pointer over the TIC graph then click the right mouse button and select unzoom from the menu. The following image shows the right click popup menu.

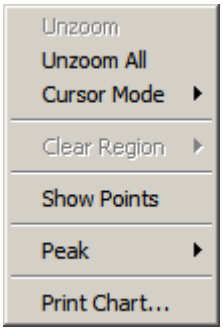


Figure 5-49 Right click mouse menu for unzoom function

There are two modes of unzoom. The **Unzoom** function steps the zoom back one step. The **Unzoom All** function returns the graph to a completely unzoomed state.

b. **Summed Select:** When the cursor is set to this mode it is only functional in the **TIC**. In all of the other graphs the cursor still functions in the zoom mode. To select an area use the mouse to drag a box over the area of the **TIC** you want to sum. A yellow box will be visible on the TIC. Each mass associated with the scans in the highlighted area will be added together and can be displayed by opening the Summed graph.

   To clear the selected region, place the cursor in the yellow highlighted area by clicking on the area with the mouse. Then click the right mouse button to open the right click menu. Then select **Clear Region** and choose either **Under Cursor**, **Summed** or **All** option to clear the selected area. The **Under Cursor** option only clears the region where the cursor line is located. If the cursor is not in a highlighted region than choosing the **Under Cursor** option will not have any effect. The **Summed** option will clear all of the yellow **Summed** regions but will leave the blue **Background** regions. The **All** option clears all selections regardless of type. The following image shows the right mouse click dialog box with the **Clear Region** menu expanded.

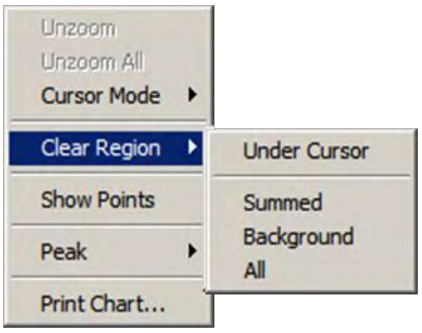


Figure 5-50 Data Review right click dialog with Clear Region menu expanded

a. **Background Select:** When the cursor is set to this mode it is only functional in the **TIC**. In all of the other graphs the cursor still functions in the zoom mode. To select an area use the mouse to drag a box over the area of the **TIC** you want as background. A blue box will be visible on the TIC. Each mass associated with the scans in the highlighted area will be added together and can be displayed by opening the **Background** graph.

   To clear the selected region, place the cursor in the blue highlighted area by clicking on the area with the mouse. Then click the right mouse button to open the right click menu. Then select **Clear Region** and choose **Under Cursor**, **Summed** or **All** option to clear the selected area. The **Under Cursor** option only clears the region where the cursor line is located. If the cursor is not in a highlighted region than choosing the **Under Cursor** option will not have any effect. The **Summed** option will clear all of the yellow **Summed** regions but will leave the blue **Background** regions. The **All** option clears all selections regardless of type. The following image shows the right mouse click dialog box with the **Clear Region** menu expanded.

13. The following image shows the last buttons on the Data Review button bar.

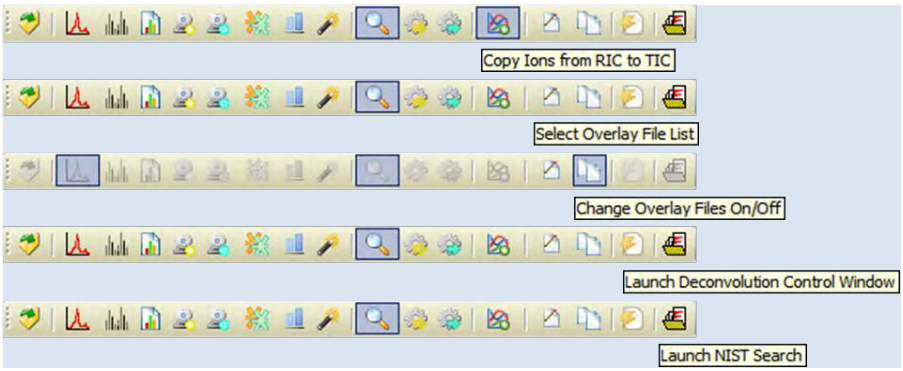


Figure 5-51 Copy Ions from RIC to TIC, Select Overlay File List, Change Overlay Files On/OFF, Launch Deconvolution Control Window and Launch NIST Search buttons

Detail on Use of Data Review Functions

RIC (Reconstructed Ion Chromatogram)

1. **Copy Ions from RIC to TIC:** If RIC ions have been added to the RIC table then clicking this button will toggle to show the RIC ions in the TIC graph or not show the RIC ions in the TIC graph. The following image shows the **Copy Ions from RIC to TIC** turned on. It also shows the color coding of the selected ions in the **MS** graph.

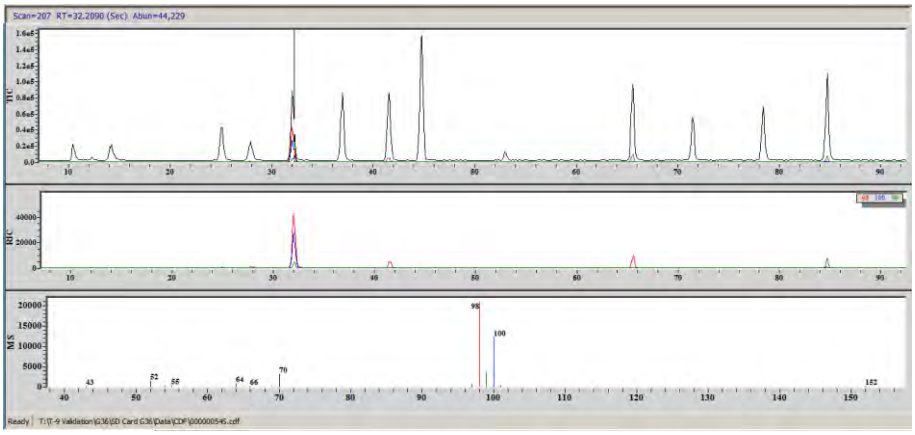


Figure 5-52 Copy Ions from RIC to TIC showing masses 98, 99 and 100

2. Selecting the **RIC Ions…** button from the Edit menu opens the following window.

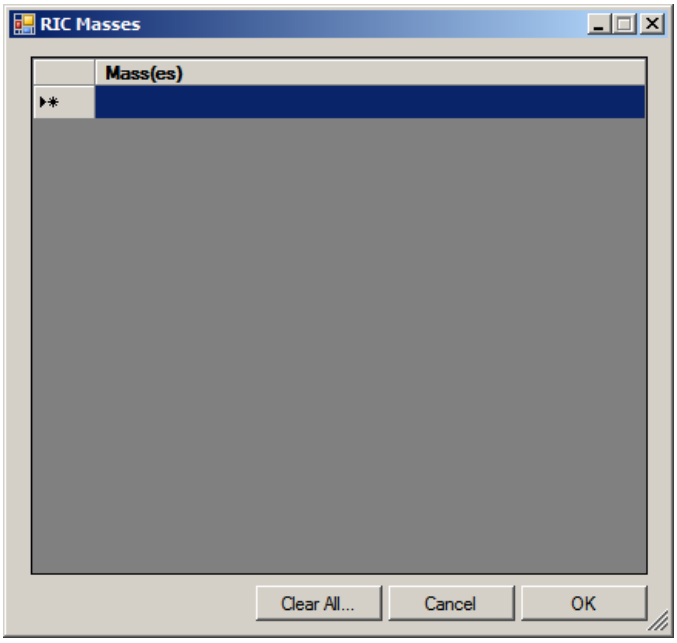


Figure 5-53 RIC Masses table

3. In this window the user can select the masses that will be shown in the RIC chart of the software. The masses are entered in by typing the mass into the blank field. They can be entered in three ways.

    a. They can be entered as an individual mass for example mass 105 would display a single trace of the intensity of mass 105 in the RIC graph chart.

    b. They can be entered in as a range of masses for example 91-93 would display a single RIC trace of the sum of the intensities of ions 91, 92 and 93.

    c. They can be entered in as a group of masses for example 91-93, 105 would display a single RIC trace of the sum of the intensities of ions 91, 92, 93 and 105.

4. To view the RIC chart first open the **View** menu from the top menu bar and select **Charts**. Ensure that the box next to RIC has been selected.

5. The masses used in a RIC trace can also be selected from the main window by using the right click menu to open a pop up dialog box in the RIC display chart. The following shows the menu used to turn RIC selection on and off.

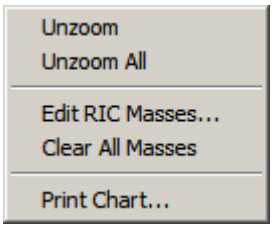


Figure 5-54 RIC edit masses right click popup menu

6. In addition to the popup menu having the RIC display window open also enables RIC selection from the MS chart.

7. With RIC graph open the user can add ions to the RIC table by simply clicking on the mass in the **MS** chart.

8. Using the menu the user can open the RIC table to see and edit the list of the selected ions.

9. CHROMION-AP shows the selected ions as colored numerical references along the top edge of the RIC graph window. This is shown below with a mass of 272 being shown in the RIC window and in the box in the top right corner of the RIC graph. It is color coded to assist in identifying the trace in the RIC chart and the selected ion in the MS chart.

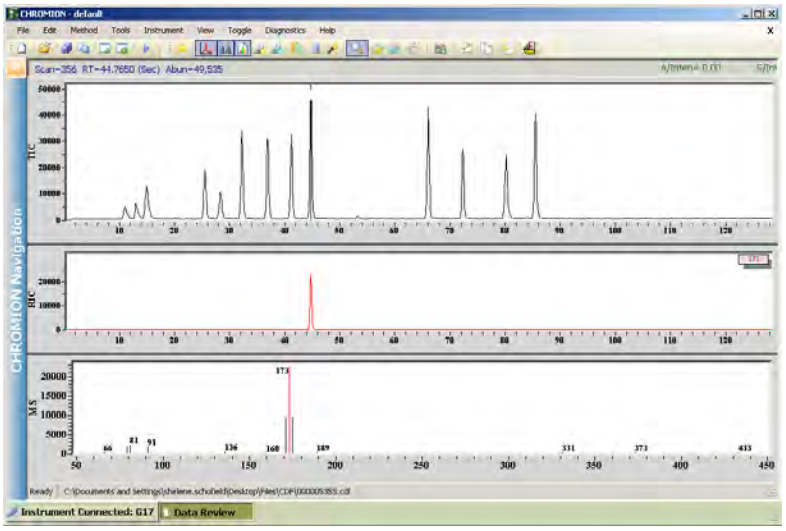


Figure 5-55 RIC ion selection from MS graph

10. To remove ions from the screen right click on RIC graph to open the popup menu. From the menu the select clear all masses to delete them from the RIC masses table or the RIC Masses table can be opened and edited.

Overlay Files

1. **Select Overlay File List:** This opens a dialog box that allows the user to select files that will be displayed in the overlay files graph.

2. Selecting the **Overlay Files…** button opens the following window.

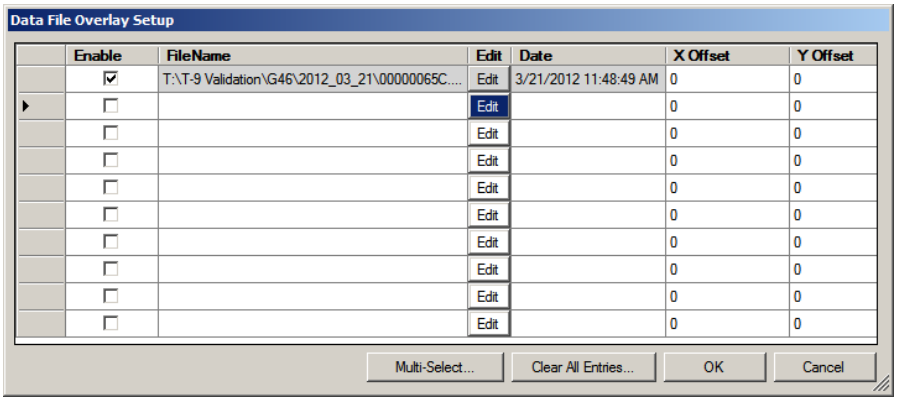


Figure 5-56 Data File Overlay Setup table

3. This window allows the user to choose which data files to overlay. Overlaying data files allows the user to view the data in a way that the user can see subtle differences between two or more data files.

4. The **Enable** check box allows the user to turn off and on the visibility of a data file in the overlay view window without removing it from the file list.

5. The **Edit** button allows the user to select a single data file to include in the overlay view window. The first line in the table shows the path and name of the currently open data file. Another file can be added by clicking the **Edit** button. The Windows open file dialog box will open and the user can then navigate to the location of the data file they want to view in the overlay screen. After selecting the file click the open button to add the file to the list.

6. The **Multi-Select…** button opens the following window.

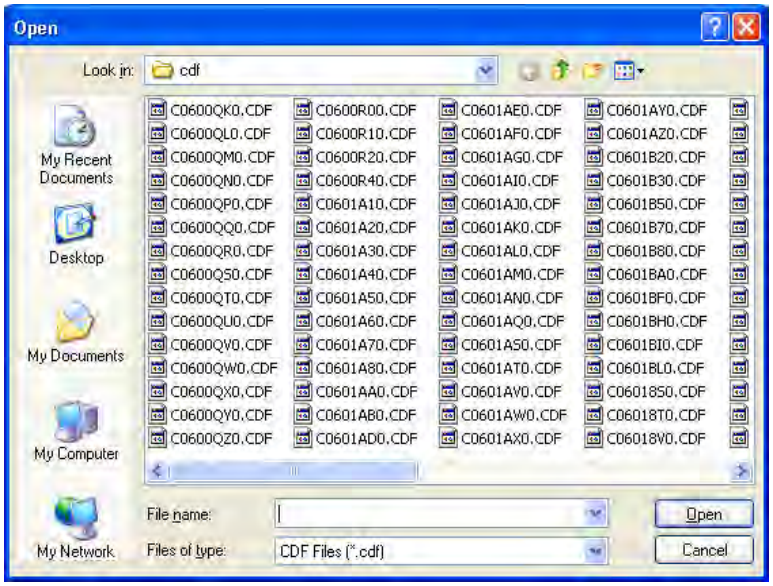


Figure 5-57 File window used to select multiple data files for display in the overlay graph

7. From this window the user can select and insert multiple files into the overlay file table. To select multiple files click the **Multi-Select…** button at the bottom of the window. Navigate to the location of the files that are to be added to the table. Click on the name of the first file to be added to the table. Then while holding the shift key click on the name of the last file to be added to the table. Alternatively while holding the control key down click on the names of files you want added to the table. After the files names have been highlighted click the open button to add them to the table.

8. To remove a file from the table right click the mouse on the name of the file that is to be removed and select remove file from the popup menu.

9. The **Date** column shows the data that the file was created.

10. The **Clear All Entries…** button removes all of the file names from the table except the original file that was open when the overlay menu was opened.

11. The **X Offset** allows the user to move a files starting time location to adjust the alignment with other TICs that are being overlaid.

12. The **Y Offset** allows the user to move a files intensity to adjust the alignment with other TICs that are being overlaid.

13. The **Cancel** button returns the user to the default graph window view of AP.

14. The **OK** button opens the overlay window view shown below.

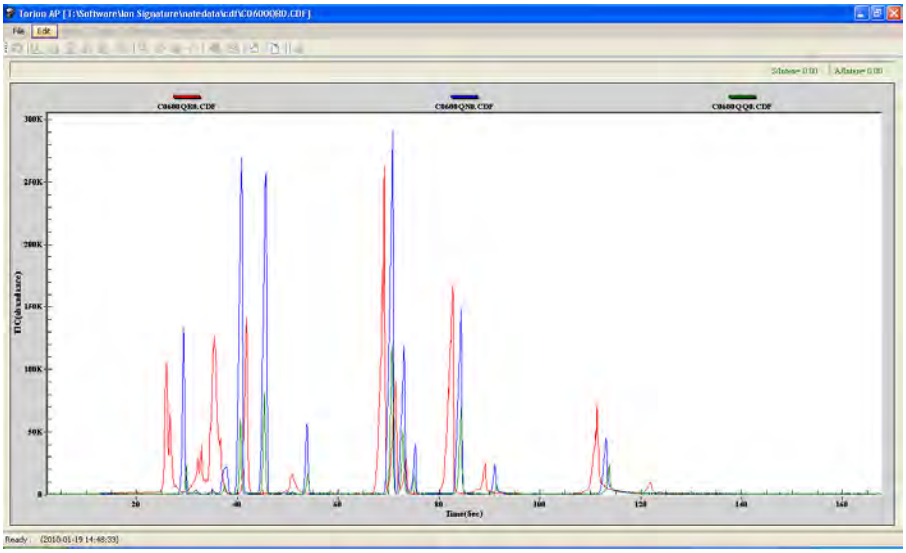


Figure 5-58 CHROMION overlay view window

15. The user exits out of this window by pressing the overlay files **On/Off** button on the button bar, which looks like two overlaying pieces of paper.

16. The user can also return to the **Overlay Files** selection window to turn on and off the overlaying function.

Deconvolution

1. **Launch Deconvolution Control Window:** Clicking this button launches the **Deconvolution Control Center**. This window is used to display and interact with data that have been deconvolved.

2. The following image shows the **Deconvolution Control Center**.

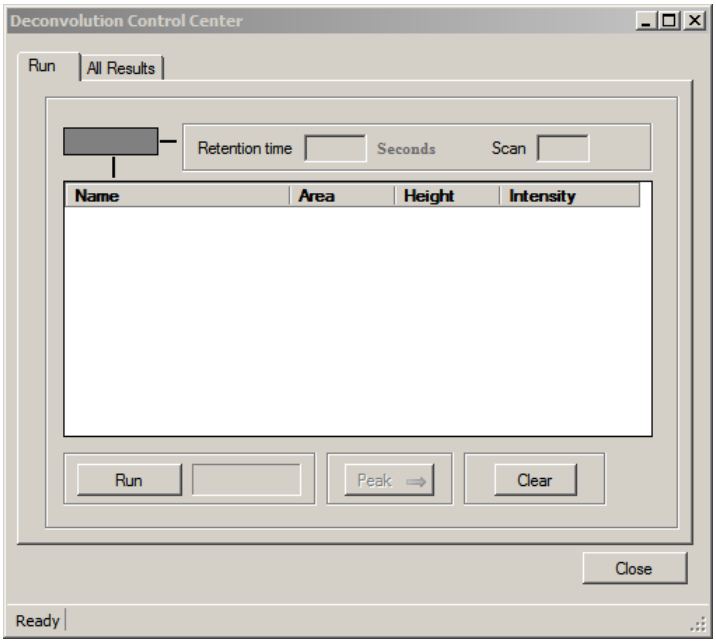


Figure 5-59 Deconvolution Control Center Run Tab

3. The **Deconvolution Control Center** uses the settings from the **Target List** and **Target List Deconvolution Parameters** to extract the spectra for a specified peak.

4. To extract the spectra press the run button at the bottom of the control window.

5. The following shows the TIC window after the spectra have been extracted.

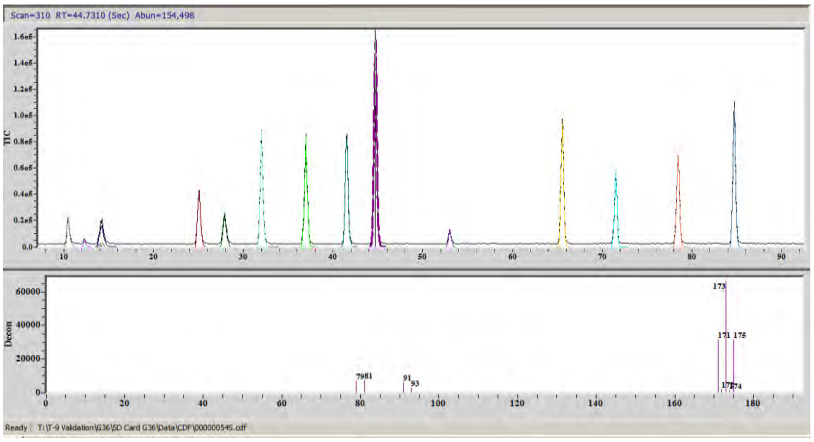


Figure 5-60 TIC with color coded peaks and spectra after a deconvolution

6. The image above shows the cursor positioned on bromoform. The peak outline is highlighted and the colored spectra are visible in the deconvolution (**Decon)** graph.

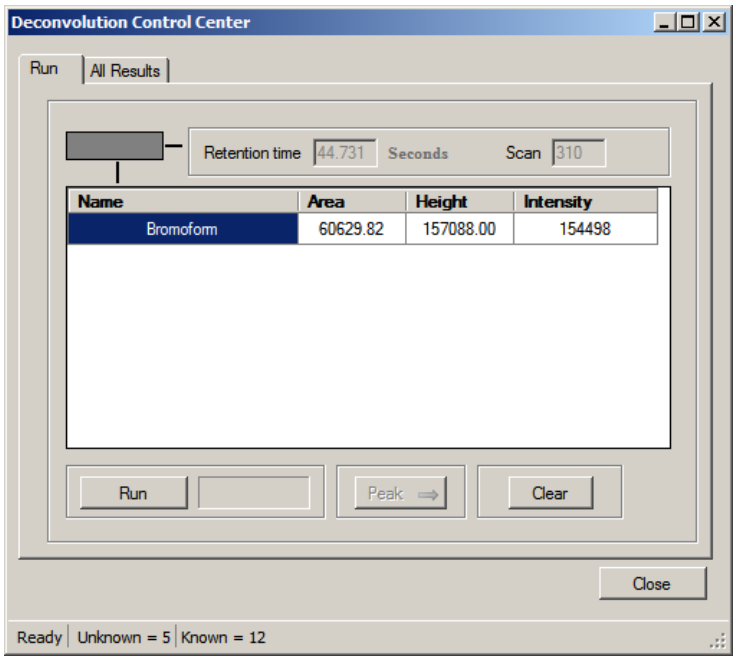


Figure 5-61 Deconvolution Control Center with bromoform selected

1. If a peak is in the **Target List** it will be identified and the when the cursor is place on the peak in the **TIC** graph the name of the peak will be shown in the **Deconvolution Control Center**. The area is the sum of the intensities of the ions that have been included in the deconvolved peak multiplied by the scan to scan difference in time. The height is the height of the deconvolved peak ions and the intensity is the height of the selected scan.

2. The following image shows a highlighted peak that is not in the **Target List.**

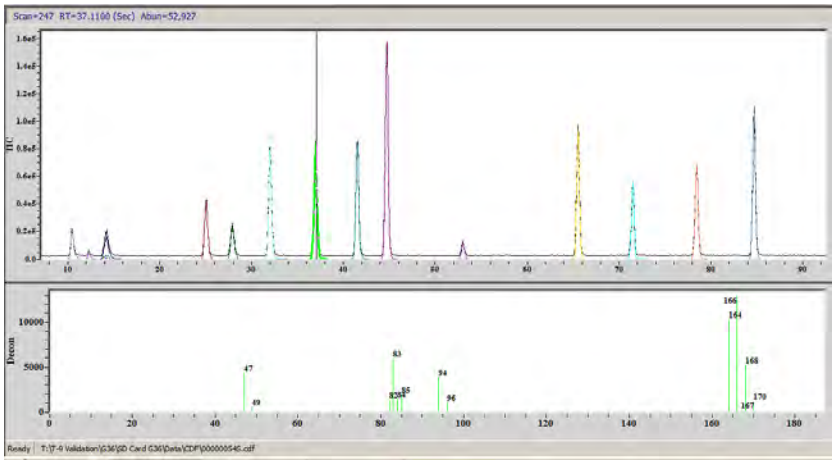


Figure 5-62 Deconvolved data with an unknown peak highlighted

3. When a peak that is not in the Target List is selected the Deconvolution Control Center will display Unknown and then a number. The number part of the label is random. In the **Deconvolution Parameter** tab in **Target List** the user can specify the number of unknown peaks to show. This is to maintain the speed of analyzing the sample when on the instrument. If a complex sample is analyzed and it has a larger number of unknown compounds the processing can be very long. By limiting the number of unknown peaks that are allowed to the 10 largest then the on instrument processing can still be kept reasonable.

If a large number of unknowns is expected and the intention is to obtain good search results for as many of the unknown compounds as possible then this setting can be increased to allow the software to deconvolved all of the unknown peaks.

4. The following image shows the **Deconvolution Control Center** with the unknown peak highlighted.

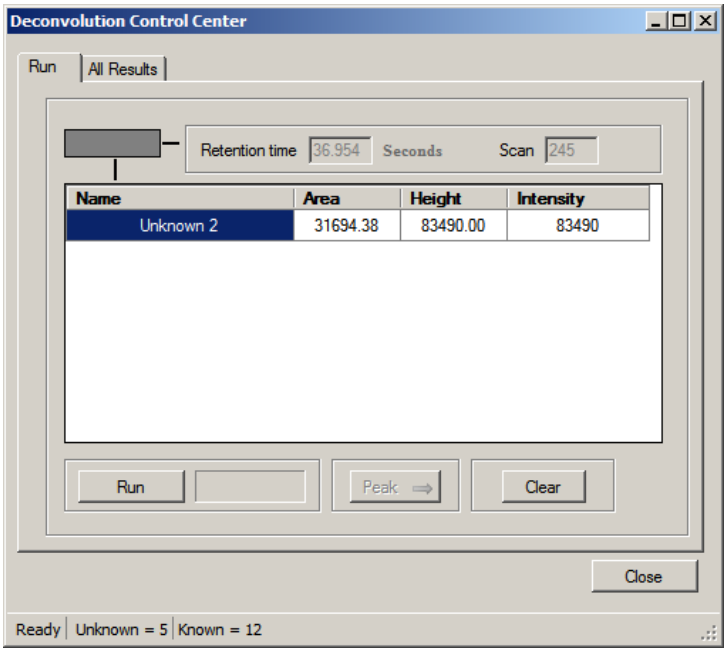


Figure 5-63 Deconvolution Control Center with Unknown peak 2 selected in the TIC

5. The area is the sum of the intensities of the ions that have been included in the deconvolved peak multiplied by the scan to scan difference in time. The height is the height of the deconvolved peak ions and the intensity is the height of the selected scan.

6. Selecting the **All Results** tab opens the following table

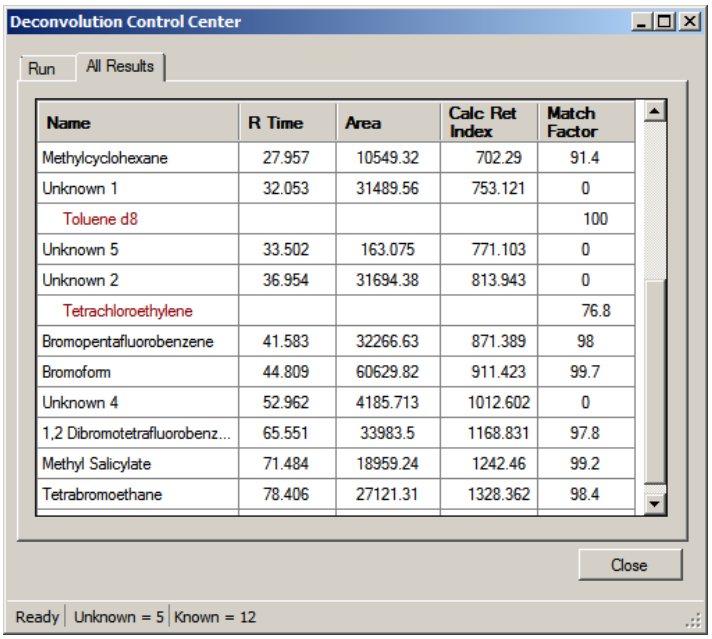


Figure 5-64 Deconvolution Control Center All Results tab showing unknown 2 identified as tetrachloroethylene

7. The unknown peaks are compared to the unknown library that is selected in the **Deconvolution Parameters** tab in the **Target List**. The number of possible peaks that will be is set in the Deconvolution Parameters tab. The possible matches are sorted on **Match Factor.**

8. The following image shows the Unknown 3 peak showing three possible matches. The correct match is acetone.

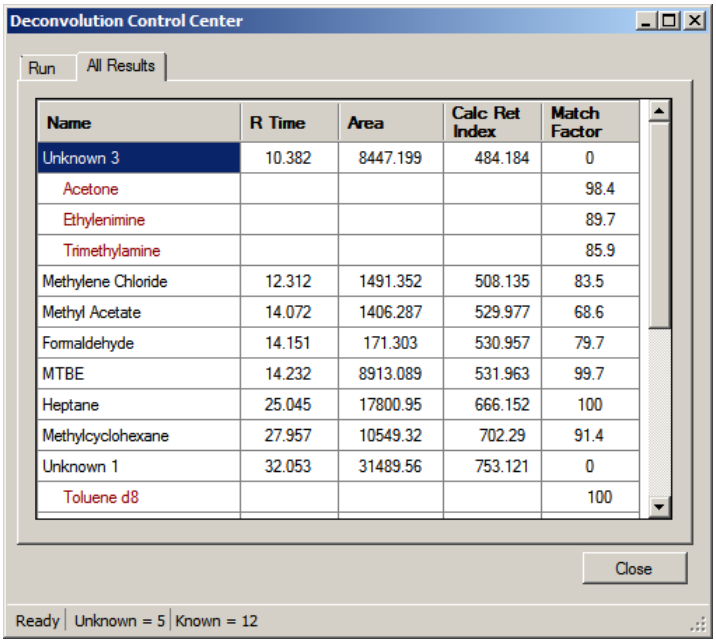


Figure 5-65 Deconvolution Control Center showing the All Results tab with multiple possible unknown matches for the peak labeled Unknown 3

9. The following image shows a TIC with three peaks two of the peaks co-elute at 53-54 seconds. Deconvolution has been performed and three peaks have been detected.

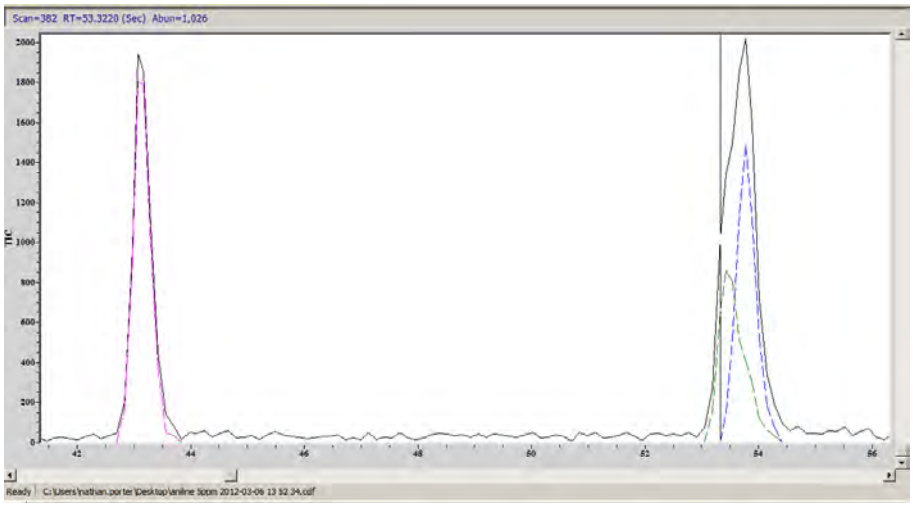


Figure 5-66 Deconvolution of three peaks with two co-eluting peaks

10. The following image shows the results of the unknown search of the deconvolved peaks.

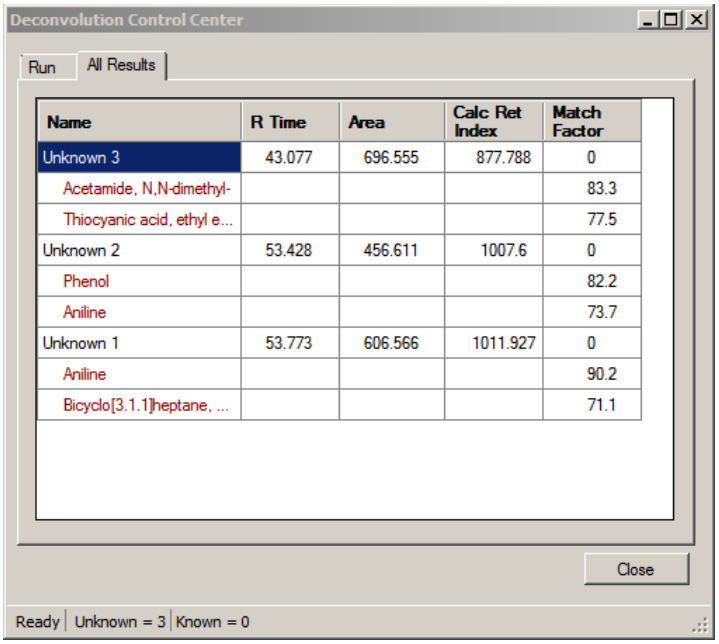


Figure 5-67 Deconvolution Control Center showing the All Results tab for three peaks identified in the unknown library. Unknown 2 and Unknown 3 are co-eluting peaks

11. The compounds are shown with the top hits for each.

NIST Search

1. **Launch NIST Search:** Clicking this button launches the NIST library search software.

2. In each of the following graphs there is an option to send spectra to a file that can be opened in the NIST MS Search software.

    a. MS

    b. Summed

    c. Background

    d. Difference

    e. Deconvolution Spectra

3. The following image shows the dialog box that opens when right clicking in the MS graph.

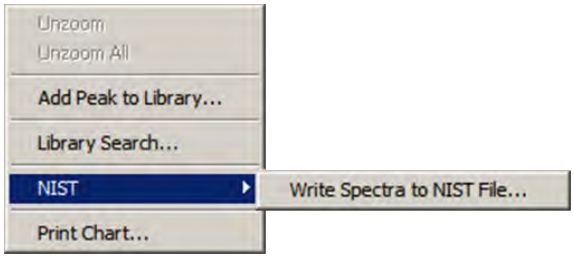


Figure 5-68 Right click menu on the MS graph Showing Write Spectra to NIST File…

4. The following image shows the dialog box that opens when the **Write Spectra to NIST File…** option is selected.

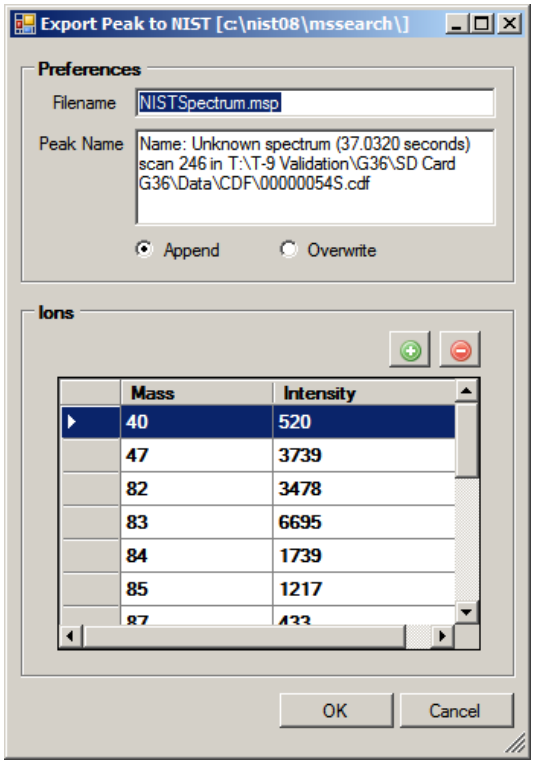


Figure 5-69 Write Spectra to NIST File... dialog box

5. The file name is the default file name set in the **Preferences** under the **Edit** menu. The name can be changed from this screen. The new name will be saved in the **Preferences** menu.

6. The masses can be edited before being sent to the file.

7. To remove an Ion, select it by clicking on the mass with the mouse. Then click the red button with the minus sign and the mass will be removed. There are no dialog boxes to warn that a mass will be removed. If a mass is removed that the user did not want removed select cancel to close the dialog box and reselect the send spectra to NIST to reopen the dialog box with the original spectral content.

8. To add a Mass, click the green button with the plus sign. This will add a blank line at the end of the table. Type in the new mass with its relative intensity.

9. The **Append** adds the spectra to the last created file as a new spectra. The **Overwrite** option replaces the file with the single spectra. This allows the operator to send multiple or single spectra to the NIST file for viewing in the NIST MS Search software.

10. After selecting the OK button the following image shows the dialog box that is displayed indicating that the spectra have been written to the file.

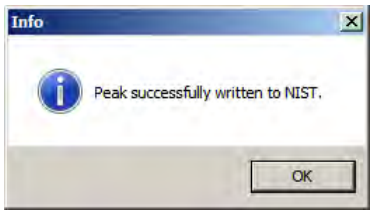


Figure 5-70 Peak successfully written to NIST file dialog box

11. Clicking the Launch NIST Search button will open the NIST MS Search software and allow the user to compare the saved spectra to the NIST data base.

Exporting Charts

1. **Export Charts:** This opens the following dialog box.

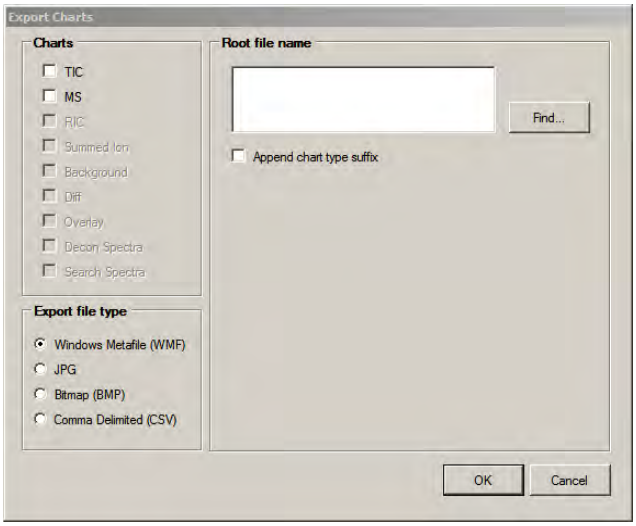


Figure 5-71 Export Charts dialog box active charts are not grayed out. Inactive charts are grayed out and not available to create images

12. To create an image place a check mark in the boxes by the type of chart you want. The following is a list of the different types of charts. More detail on how to get these charts and what they are used for will be given latter in this section of the manual.

    a. **TIC:** Total Ion Chromatogram. This is the GC trace of the entire signal that is generated by the detector in the mass spectrometer.

    b. **MS:** Mass Spectra. This is the spectra for a single scan in the TIC.

    c. **RIC:** Reconstructed Ion Chromatogram. This is the chromatographic trace for selected masses and can be used to look for a specific peak with a given mass.

    d. **Summed Ion:** This is the spectra of a group of chromatographic scans that have been selected using the average function.

    e. **Background:** This is the spectral data for a section of background selected by the user.

    f. **Diff:** This is the spectral data showing the difference between the background spectra and the highlighted section of chosen spectra.

    g. **Overlay:** This is a chromatographic trace of several TICs that have been selected and are displayed together in the same chart.

    h. **Decon Spectra:** This is the spectral graph of the deconvolution peaks.

    i. **Search Spectra:** This shows the head to tail spectra of an unknown compound search. The spectra from the library are on the bottom and the spectra from the analytical run are on top.

13. The charts can be exported as WMF, JPG, BMP or CSV files. One of these options needs to be selected in the Export File Type box.

14. The **Find** button allows the user to enter a file name and to select the location where the image files will be stored after they are created.

15. The **Append Chart Type Suffix** option when checked adds the .wmf, .jpg, .bmp or .CSV extension to the file name.

16. The CSV data are saved in two columns with the time first and the response second. In the case of overlaid TICs the data are in two columns with the time starting at zero then progressing to the end of the first file. The time then returns to zero and starts the with the data from the next file. This is repeated until all of the files in the overlay graph have been stored in the CSV file. The data can be plotted as one single plot. The data cannot be easily plotted side by side since the retention time of the data points is not a fixed time. Therefore each set of data will have different times on the x axis. This is a result of the dynamic ionization used in the toroidal ion trap.

Mass Spectrometer

1. The Mass Spectrometer screen is where the settings that control the instrument are configured and sent to the instrument. It is also where the data for mass calibration are stored.

2. These settings are not included in the method because they are specific to the instrument. Methods can be transferred between instruments while the Mass Spectrometer settings cannot.

3. It is not recommended that most of these setting be changed. Recommended default values are given in the Advanced Operations section of this manual. Read the entire chapter before making any changes to the mass spectrometer settings.

Caution!

Changing setting on the mass spectrometer without proper training may cause damage to the instrument and may result in costly repairs. Only adjust these setting if you have a complete understanding of what the setting is used for and what it does.

4. The button bar in the Mass Spectrometer screen allows the user to backup the settings for an instrument before making changes. For the reasons stated in the above caution the settings from one instrument should not be loaded onto a different instrument.

5. The following image shows the button bar for the **Mass Spectrometer** screen.

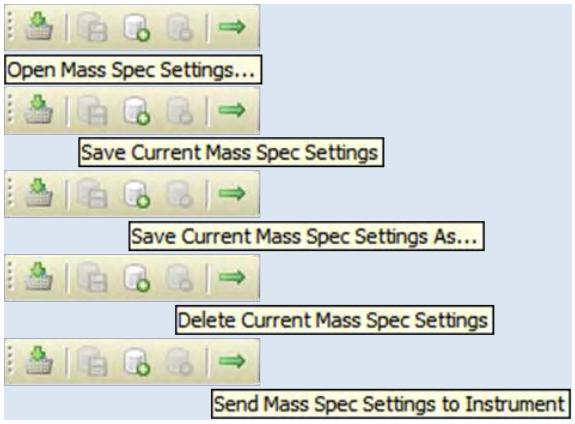


Figure 5-72 Mass Spectrometer screen button bar

a. **Open Mass Spec Settings…**: This allows the user to load previously saved settings into the Mass Spectrometer table. It is also used to update the displayed data. The following image shows the dialog box that opens when opening mass spec settings.

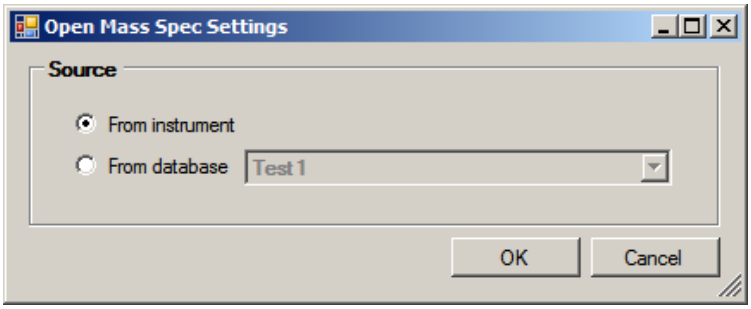


Figure 5-73 Open Mass Spec Settings... dialog box

When the **From instrument** option is selected the table will be updated from the currently connected instrument. The **From database** option allows the user to select saved settings to load into the table.

b. **Save Current Mass Spec Settings…**: This option allows the user to save the currently displayed settings to the current settings database entry. This option is only available when

a settings table has previously been saved. The name of the saved table is displayed in the blue bar at the top of the **Mass Spectrometer** screen just below the button bar.

c. **Save Current Mass Spec Settings As…**: This button is used to save the settings and provide the database entry with a name. If the settings table has been saved previously this button allows the user to give the settings table a new name. The following image shows the dialog box.

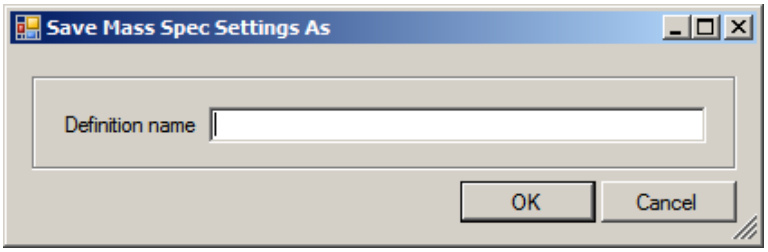


Figure 5-74 Save Mass Spec Settings as dialog box

d. **Delete Current Mass Spec Settings**: This button deletes the open settings table. If the current table is the one that is on the instrument this option will not be available.

e. **Send Mass Spec Settings To instrument:** This will send the currently displayed settings to the instrument. This action is immediate and cannot be undone. Most of the settings will take immediate affect even if the instrument is performing an analysis. This can useful for diagnostic purposes but as described in the previous caution sending parameters without understanding what they do can cause damage to the instrument.

6. The only settings that normally need to be adjusted are the following.

a. **Hard Solvent Delay**: The hard solvent delay allows the user to turn off the mass spectrometer until a large solvent peak has eluted from the column. This helps keep the instrument clean and keeps the visual scale of the peaks reasonable during the analysis.

To turn on the hard solvent delay find the following settings. In the group **MassSpectrometer** find the **Subgroup IonSource. HardSolventDelay** is the first choice. Enter the time that the filament will be left off at the start of the run. Typically 5 to 10 seconds. Next find the **Subgroup MassAnalyzer. HardSolventDelay** is the first item. Enter the same time as that set in the **IonSource HardSolventDelay.** Next find the **Subgroup Detector**. **HardSolventDelay** is the second item in this **Subgroup** set this time to the same value as the other two times.

b. **Detector Voltage**: The detector is an electron multiplier. These detectors degrade over time. To maintain the performance of the instrument it is necessary to change the voltage on the detector. For inexperienced users it is suggested that the changes be made using the **Tuning Wizard** in the software. The setting can be changed by entering the desired value in the **MassSpectrometer Group Detector Subgroup** and the **HighVoltageVoltage** field. Normal operating range is -1200 to -2200. Inappropriate values will result in poor performance of the instrument.

c. **Filament Current**: The filament is used to create electrons. The electrons are used to ionize the analytes. The filament degrades over time. To maintain the performance of the instrument it is necessary to change the current on the filament. For inexperienced users it is suggested that the changes be made using the **Tuning Wizard** in the software. The setting can be changed by entering the desired value in the **MassSpectrometer Group IonSource**

Subgroup and the **FilamentCurrent** field. Normal operating range is 0.85 to 1.2. Inappropriate values will result in poor performance of the instrument.

File Manager

1. The **File Manager** is similar to Windows file management. It is intended as a safe way to transfer files to and from the instrument SD card.

2. From the file manager the user can create a directory on the connected computer and can move data files to the computer from the SD card. The types of files have been described earlier. They are:

    a. **.RES**: These contain all of the results of an analysis including the data and the libraries, settings and reports that were generated or used during an analysis. It is highly recommended that these be the files moved to the computer.

    b. **.Zip**: These are the results files for **Performance Validation** runs and are used in the **Tuning Wizard**. Like the .RES files they contain all of the information used and generated during a **Performance Validation** run.

    c. **.CDF**: This is the data that has been converted to usable searchable data. These files are contained in the **.RES** file.

    d. **.RAW**: This is the unconverted data that is gernerated by the instrument. These files are contained in the **.RES** file.

    e. **.TXT**: These are a text report file generated during an analysis. The same data as that shown on the instrument front panel is contained in this file. These files are contained in the **.RES** file.

3. The following image shows the **File Manager**.

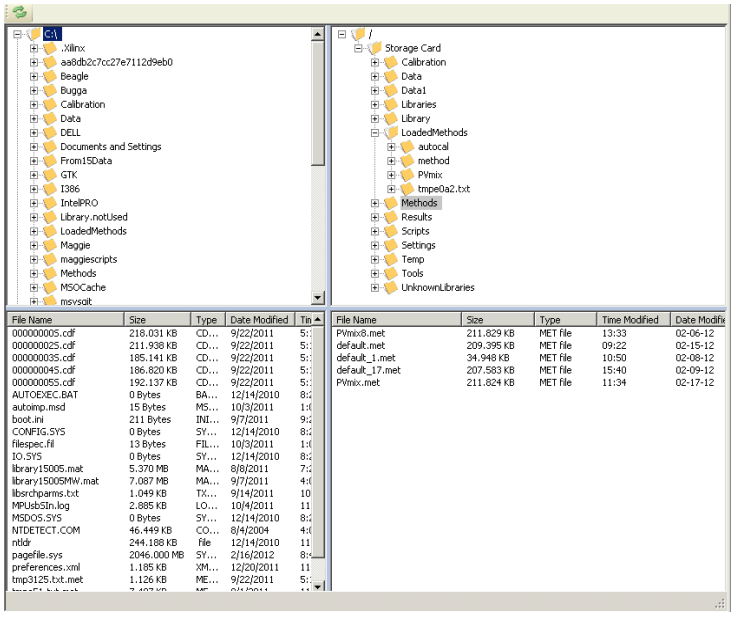


Figure 5-75 File Manager

4. Create a data folder on the computer by right clicking on the computer drive C:\ or a sub folder of C:\. The following image shows the create folder menu that open after right clicking on a folder on the left side of the **File Manger** window.

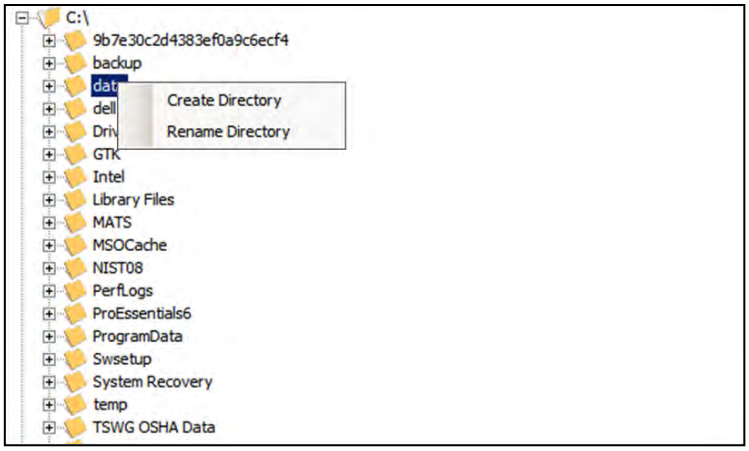


Figure 5-76 File Manager Create Directory and Rename Directory dialog box

5. Click on the name of the folder where the files are to be stored. The frame at the bottom left side of the window will display the files that are already in the folder. If it is a new folder the bottom left frame will be empty.

6. Click the plus symbol next to the top folder on the right top side of the screen. This will expand the tree view.

7. Next select the plus symbol next to the folder labeled Storage Card and the tree view will be expanded.

8. Next select the plus symbol next to the data folder. Finally expand the folder that is labeled with the date when the data were collected.

9. The data will be displayed in the bottom right frame. Click on the .RES file name that you want to move and while holding down the mouse button drag it to the bottom left frame.

10. To select multiple files click on the top file that is to be selected then press and hold down the shift key then click the bottom file that is to be selected. The using the mouse click on the highlighted files and while holding down the mouse button drag them to the left side of the screen.

11. Files can be deleted only from the bottom frames. To empty the SD card it is possible to delete files by right clicking and selecting the delete option from the popup menu.

12. To do more advanced file manipulation remove the SD card from the instrument and insert it into a computer. Then use the software on the computer to move and delete files.

Caution!

When using the **File Manager** in the CHROMION software some files and directories are protected. This prevents deletion of items that are important to the operation of the instrument. When viewing and editing the SD card directly on a computer none of these safeguards are in effect. To prevent loss of data it is best to create a copy of the SD card on the computer before deleting any files.

If files or folder have been deleted the firmware on the instrument will reconstruct the SD card directories but all data and libraries will not be loaded until they are sent from a computer running CHROMION.

Library Editor

1. The **Library Editor** is used to look at and change libraries. After they have been refined they can then be exported as an unknown library for use on the instrument or compounds can exported to the **Target List**.

2. The following screen shows the **Library Editor.**

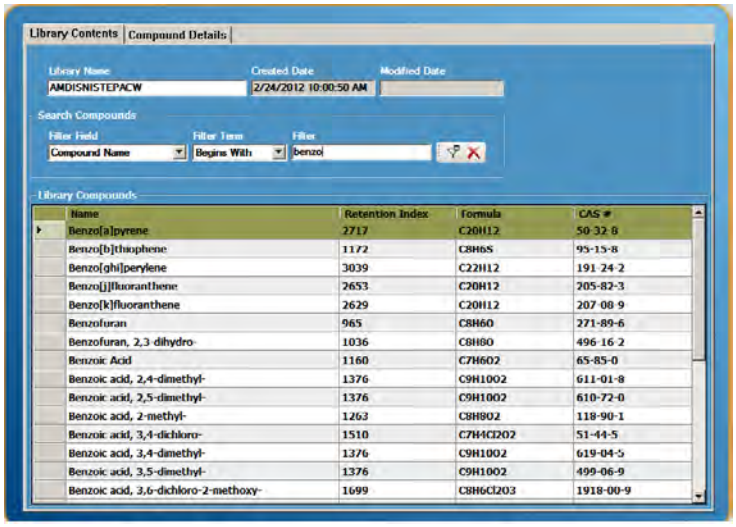


Figure 5-77 Library Editor Library Contents tab

3. The software comes with a library loaded. This library is an edited version the NIST Amdis EPA library. This library consists of data that are generated on quadrupole mass spectrometers. The unknown search algorithms in most cases work well to match the data from the ion trap to NIST libraries.

Caution!

The difference between **Target Lists** and libraries is primarily where the data came from. While it is possible to add compounds from any library to the Target List it is important to note that some library data were generated on instruments that may give slightly different spectra than the TRIDION instrument. This is because different types of mass spectrometers work in different ways.

It is usually best to generate **Target Lists** on the instrument using standards. Second best is to use compounds from libraries that have been generated using a TRIDION GC-MS instrument.

Using other libraries to create Target Lists can reduce the accuracy of the search algorithms.

a. **Library Name**: This field is used to name or rename a library as well as to see the name of the currently open library.

b. **Created Date**: This field shows the date that the library was created. This date and time comes from the computer clock and will be wrong if the clock is not set to the correct date and time.

c. **Modified Date**: This field shows the date and time that the library was last edited. This date and time comes from the computer clock and will be wrong if the clock is not set to the correct date and time.

d. **Search Compounds**: This part of the software is used to search the library. The following parts of the search option:

i. **Filter Field**: The user can select from search options.

1. **Compound Name**
2. **CAS #**
3. **Formula**
4. **Retention Index**

ii. **Filter Term**: This allows the user to select from the following terms when searching:

1. **Begins With**
2. **Contains**
3. **Ends With**
4. **Exact Match**

iii. **Filter**: This is where the user types in the characters that are to be matched.

iv. The first button executes the search. The button with the red X on it clears the search fields.

4. The following image shows the Compound Details tab:

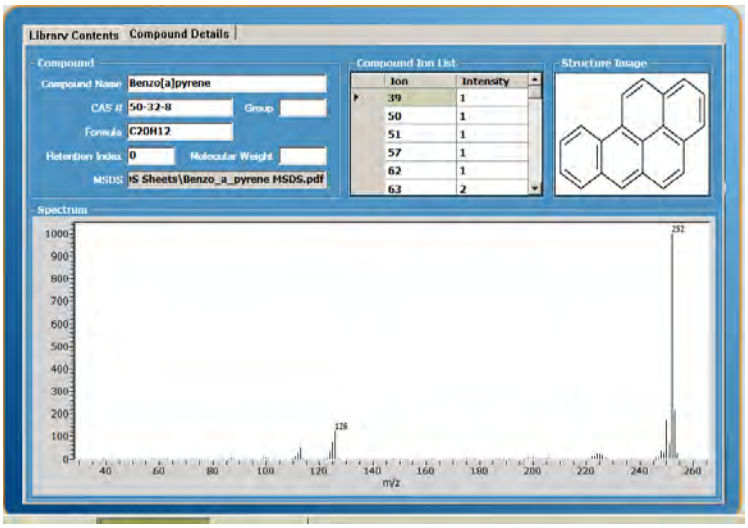


Figure 5-78 Library Editor Compound Details tab

5. The following are parts of the **Compound Details** tab:

a. **Compound**: This field contains the following information:

i. **Compound Name**

ii. **CAS #**

iii. **Formula**: Molecular formula

iv. **Retention Index**

v. **Molecular Weight**

vi. **Group**: User assigned information for sorting the compounds

vii. **MSDS**: This option allows the user to set up a link to an external file. The field displays the path to the linked file. Right clicking on the field allows the user to add a new link or remove an existing link.

The field is labeled MSDS but can be linked to any file and will use the Windows configuration to select the program that will be used to try to open the file.

b. **Compound Ion List**: This is the list of ions for the compound. They can be edited by highlighting the field and typing in a new value. The user can add or delete an ion by using the right click menu.

c. **Structure Image**: This field is used to view an image. The image can be any image that is a supported type. The supported file types are BMP, JPEG, GIF and PNG. The user can add remove or view a file by using the right click menu.

6. **Spectrum**: This is a graphical view of the information that is contained in the **Compound Ion List**. It cannot be edited and is only available for viewing.

7. The following image shows the **Library Editor** button bar with popup labels.

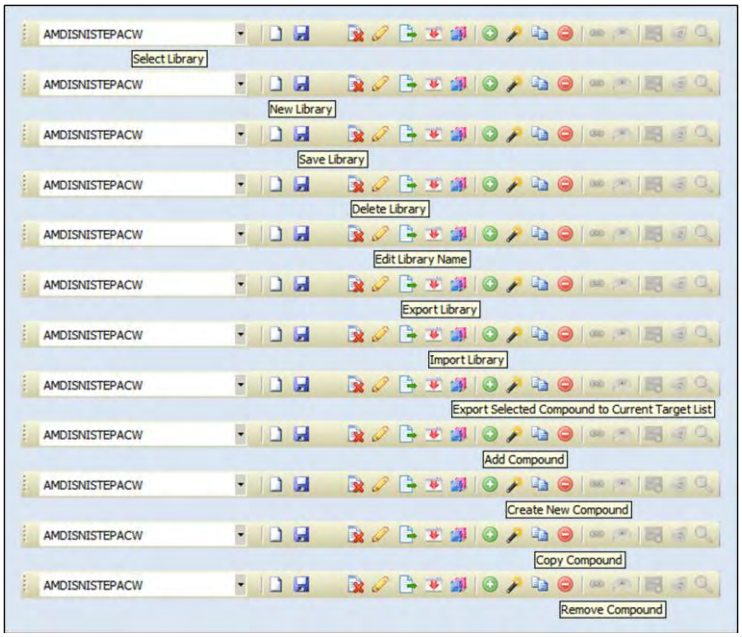


Figure 5-79 Library Editor button bar with Compound Details tab open

8. The following are the descriptions of the button bar items.

a. **Select Library**: This opens a drop down list of all of the libraries in the data base. To open a library click on it in the list.

b. **New Library**: This option creates a blank library form that can be filled in by the user. To give the library a name besides the default name type the new name into the **Library Name** field and then save the library.

c. **Save Library**: this option saves the currently open library.

d. **Delete Library**: This option deletes the currently open library. A confirmation dialog box will open to confirm that the library should be deleted. The software requires at least one active library so it is not possible to delete the last library in the list.

e. **Edit Library Name**: This option allows the user to enter a new library name for the currently open library.

f. **Export Library**: This option allows the user to export a library to a file. This library can then be loaded onto the instrument and can be used for unknown searches in the CHROMION software. See the instructions in this manual for the **Target List Deconvolution Parameters** tab for how to use the exported library files.

g. **Import Library**: This option allows the user to import a library file. This can be used to import libraries that are exported from the NIST data base or that have been previously exported from the CHROMION software.

h. **Export Selected Compound to Current Target List**: The option immediately exports the currently highlighted compound to the currently open **Target List**. To undo this action open the **Target List** and delete the compound that was just added.

i. **Add Compound**: This option opens a default library that contains a list of compounds. The user can select any of these compounds by highlighting them in the list and clicking the **Add Compound** button. The filtering options can be used to sort the default compound list. To select multiple compounds click on the name of a compound then press and hold down the shift key then click the name of the bottom compound that is to be selected. Then click the **Add Compound** button to move the compounds into the currently open library. Alternatively hold down the control key and click on the compounds to be added. Once the compounds have been highlighted click on the **Add Compound** button to add the selected compounds to the currently open library.

j. **Create New Compound**: This option creates a blank line in the compound list and opens the **Compound Details** tab for data entry.

k. **Copy Compound**: This option creates a copy of an existing compound in the **Library Compounds** table. To create a copy highlight the desired compound then click the Copy Compound button. A compound with identical information is added just below the selected compound. It has the name modified to say copy (X). The X is an incremented number that increases by one for each copy made. For example if a copy of benzene is made the new compound would be named benzene- copy (1). If a copy of toluene is then made it would be named toluene copy (2). The compound can then be renamed and edited. The columns can be sorted by clicking on the top row of the Library Compounds table. The Search Compound field can also be used to find the new compound.

l. **Remove Compound**: This option is used to delete a compound from the compound list. Select the compound by clicking on it. Then click the **Delete Compound** button. A dialog box opens allow the user to confirm that they would like to delete the compound.

9. The following image shows the **Library Editor** button bar with the **Compound Details** tab open.

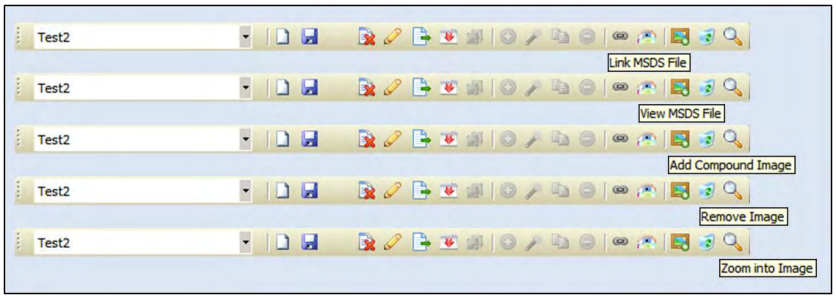


Figure 5-80 Library Editor button bar with the Compound Details tab open

10. The following are descriptions of the **Library Editor** buttons that are active when the **Compound Details** tab is open:

    a. **Link MSDS File** This option opens the following dialog box which allows the user to link a file to the Compound Details MSDS field.

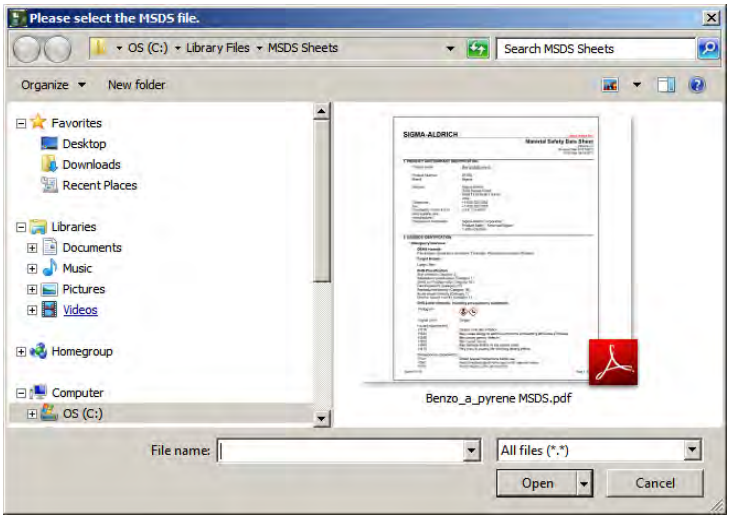


Figure 5-81 Link MSDS file location dialog

    b. **View MSDS File:** This opens the MSDS file that was linked previously.

    c. **Add Compound Image**: This opens the following dialog box that allows the user to select an image file that shows the compounds structure.

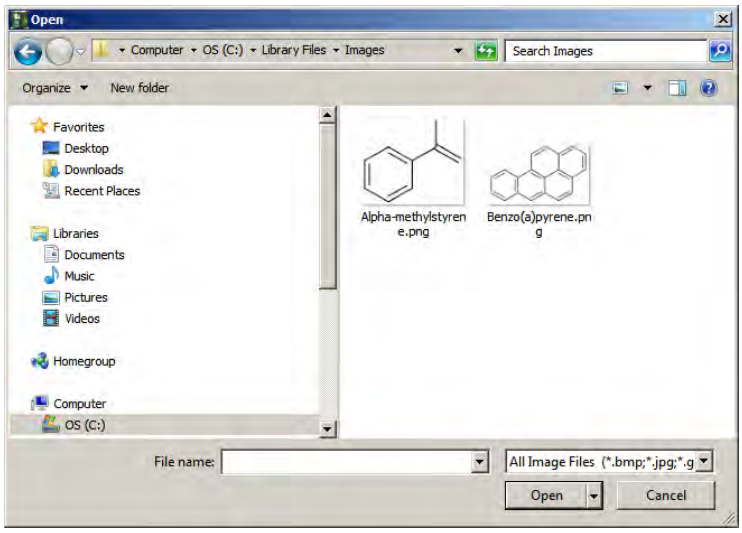


Figure 5-82 Library Editor Add Compound Image dialog box

d. **Zoom Into Image**: This option opens a larger copy of the Structure Image.

11. Almost all of the functions found on the menu bar are duplicated using the right click popup menus.

Real Time Plots

1. Real time plots are used to display information from the instrument on a computer. To display a plot the software must connected to an instrument. Information from only one instrument at a time can be displayed.

2. The following shows an image of the **Real Time Plots** screen.

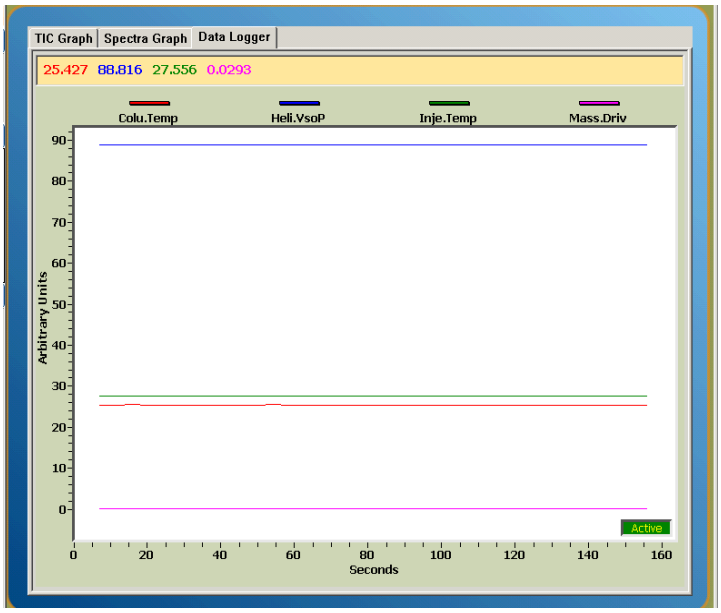


Figure 5-83 Real Time Plots screen

3. There are three types of plots.

a. **TIC Graph**: This displays the TIC in near real time as it is running on a connected instrument. The user can zoom in and out on the plot but has no control over the starting, stopping or other aspects of the data. To view the data after a run has completed the user must download the data to the computer using the **File Manager** and can then open the data using **Data Review**.

b. **Spectra Graph**: This graph shows a single scan from the last downloaded scan. Like the TIC graph the user can zoom in and out on the data but has no control of starting stopping or other aspects of the data. To view the data after a run has completed the user must download the data to the computer using the **File Manager** and can then open the data using **Data Review**.

c. **Data Logger**: The data logger is used to log selected reading from the instrument.

d. The following image shows the **Real Time Plots** button bar**.**

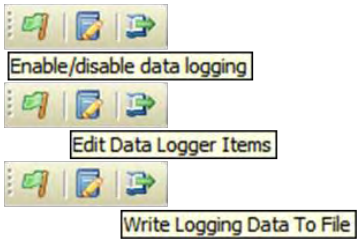


Figure 5-84 Real Time Plots button bar

e. To use the **Data Logger** feature it needs to be enabled. To turn on logging right click on the **Data Logger** window and select logging then select **Enabled** or click the **Enable/disable data logging** button on the button bar. The following image shows the popup menu that is used to enable or disable data logging.

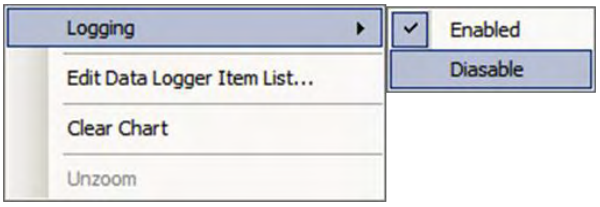


Figure 5-85 Enable Data Logger dialog box

f. Following list shows the various values that can be plotted**.** To select the items to plot right click on the Data Logger screen and select the **Edit Data Logger Item List…** option from the popup menu or click the **Edit Data Logger Items** button on the button bar

Column.Temperature	Column Temperature
Detector.HighVoltageCurrent	Electron Multiplier Detector Current
Detector.HighVoltageVoltage	Electron Multiplier Detector Voltage
Helium.HighPressure	Internal Helium Cylinder Pressure
Helium.VSOPressure	Pressure at the Head of the Column
Injector.Temperature	Injector Temperature
IonSource.FilamentBiasVoltage	Filament Barrel Bias Voltage
IonSource.FilamentCurrent	Filament Current
IonSource.FilamentGateHighVoltage	Einsel Lens High Voltage
IonSource.FilamentGateLowVoltage	Einsel Lens Low Voltage
IonSource.FilamentVoltage	Filament Voltage
MassAnalyzer.AmplitudeVoltage	RF Amplitude Voltage
MassAnalyzer.DriveCurrent	RF Drive Current
MassAnalyzer.DriveTemperature	RF Drive Temperature
MassAnalyzer.DriveVoltage	RF Drive Voltage
MassAnalyzer.StepAVoltage	RF Step A Voltage
MassAnalyzer.StepBVoltage	RF Step B Voltage
PowerSystem.AverageCurrentA	Average Current Battery Cell A
PowerSystem.AverageCurrentB	Average Current Battery Cell B
PowerSystem.AverageRemainTimeA	Average Remaining Time Battery Cell A
PowerSystem.AverageRemainTimeB	Average Remaining Time Battery Cell B
PowerSystem.AverageTimeToChargeA	Average Time To Charge Battery Cell A
PowerSystem.AverageTimeToChargeB	Average Time To Charge Battery Cell B
PowerSystem.BatteryCurrentA	Battery Cell A Current
PowerSystem.BatteryCurrentB	Battery Cell B Current
PowerSystem.BatteryVoltageA	Battery Cell A Voltage
PowerSystem.BatteryVoltageB	Battery Cell B Voltage
PowerSystem.CaseTemperature	Internal Instrument Temperature
PowerSystem.Cpu33Voltage	CPU Power 3.3 V
PowerSystem.CurrentOutMonitor	Power Board Total Current out
PowerSystem.MainVoltage	Main System Voltage
PowerSystem.Negative15Voltage	Power Board – 15 V
PowerSystem.Negative5Voltage	Power Board -5 V
PowerSystem.Positive10Voltage	Power Board 10V
PowerSystem.Positive15Voltage	Power Board 15V
PowerSystem.Positive24Voltage	Power Board 24V
PowerSystem.Positive26Voltage	Power Board 26V

PowerSystem.Positive33Voltage	Power Board 3.3V
PowerSystem.Positive5Voltage	Power Board 5V
PowerSystem.RemainCapacityA	Battery Cell A Remaining Capacity
PowerSystem.RemainCapacityB	Battery Cell B Remaining Capacity
PowerSystem.RemainPercentA	Remaining Percent of Charge left in Battery Cell A
PowerSystem.RemainPercentB	Remaining Percent of Charge left in Battery Cell B
PowerSystem.RemainTimeA	Remaining Time Left For Battery Cell A
PowerSystem.RemainTimeB	Remaining Time Left For Battery Cell B
PowerSystem.TemperatureA	Battery Cell A Temperature
PowerSystem.TemperatureB	Battery Cell B Temperature
PowerSystem.VoltageInMonitor	Voltage Coming In From Wall Power
RoughingPump.Current	Current Being Drawn By Roughing Pump
TransferLine.Temperature	Transfer Line Temperature
TrapHeater.Temperature	Ion Trap Assembly Temperature
TurboPump.BearingTemperature	Turbo Pump Bearings Temperature
TurboPump.BottomTemperature	Turbo Pump Temperature at Bottom of Housing
TurboPump.Current	Current being Drawn By The Turbo pump
TurboPump.ElectronicsTemperature	Turbo Pump Electronics Temperature
TurboPump.MotorTemperature	Turbo Pump Motor Temperature
TurboPump.Speed	Turbo Pump Speed
VacuumChamber.Pressure	Vacuum Pressure Reading

g. The following image shows the **Data Logger Items** dialog box.

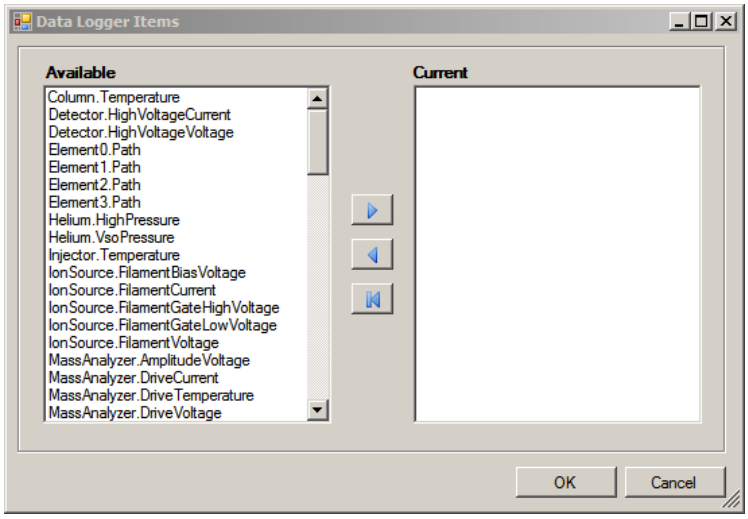


Figure 5-86 Real Time Plots Data Logger Items dialog box

h. Select the item to be plotted from the **Available** side of the dialog box and click the top blue arrow to move the selected item to the **Current** side of the dialog box.

i. Items can be removed from the **Current** side of the dialog box by selecting them with the mouse and using the second arrow button to move the selected item back to the **Available** side of the dialog box.

j. All of the items in the Current side of the dialog box can be moved back to the Available side of the dialog box by clicking on the bottom blue arrow.

Note

Selecting items to plot that have large differences in value, for example **Electron Multiplier Detector Voltage** that typically has a signal of -1200 to -2200 and **Power Board 3.3V** that will have a signal of 3.1 to 3.4 will result in scaling that makes the **Power Board 3.3V** reading useless.

4. To save the data to a CSV file. Disable the data logger using either the right click menu or the button on the button bar. The click the **Write Logging Data To File** button on the button bar. The save file Windows dialog box will open. Navigate to the location where the file is to be saved and enter the name of the file then click on OK.

Tuning Wizard

1. The Tuning Wizard is used to check the performance of the GC-MS.

2. The following shows the Tuning Wizard screen.

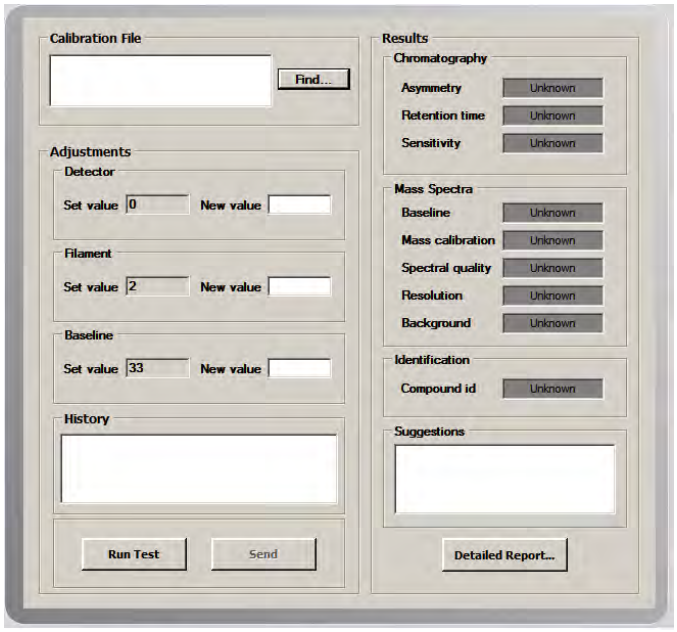


*Figure 5-87 Tuning Wizard screen*files that are updated automatically when a new version of CHROMION is installed

3. For more advanced users it is possible to use customized INI and library files. To open the file location dialog box click on the **Select Location of INI File** button. This button is shown in the following image.

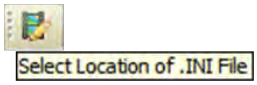


Figure 5-88 Tuning Wizard button bar

4. The Tuning Wizard Files dialog box will open. The following image shows this dialog box.

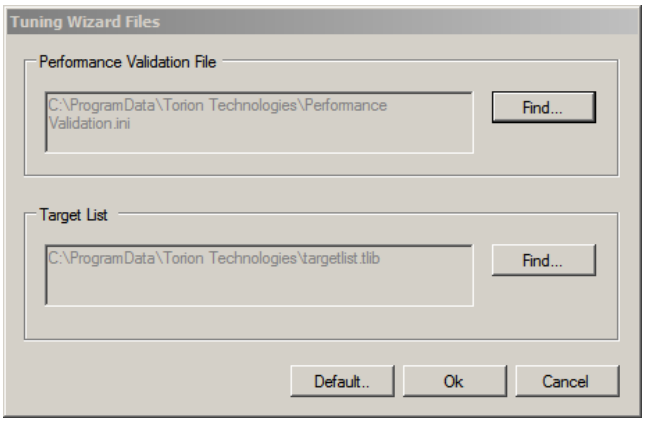


Figure 5-89 Tuning Wizard Files dialog box

5. The files are custom and can be save in any location. The only requirement is that they be in the correct file and that the Performance Validation File be saved with an INI file extension and the library file be saved with a tlib file extension.

6. If a file location has been specified that location will still be specified when a new copy of CHROMION is installed. To Change back to the default files select the **Default** button. Contact Torion for more details on making and using custom INI or library files.

7. To check the performance of an instrument it is necessary to run a performance validation analysis on the instrument. Instructions on running a performance validation are described in Chapter 4.

8. After running the performance validation use the **File Manger** to move the Calibration Results file to the computer. The calibration results are saved in the following folder on the instrument storage card.

   /Storage Card/Calibration/Results.

9. The performance validation results files have a .zip file extension. They are archived on the storage card by date. It is important to make sure that the most recent file is the one moved to the computer.

10. Load the file into the Tuning Wizard by clicking the **Find** button in the **Calibration File** frame located at the top left of the **Tuning Wizard** screen. The Windows open file dialog box will open. Navigate to the location of the calibration file and click on it to select it then click open to load the file into the **Tuning Wizard**.

11. Click the Run Test button to check the performance of the instrument.

12. The results are displayed in an easy to read format. The detailed report shows more information about the tests and the results. Some of the tests shown in the detailed report are grouped into the results on the main screen.

13. If a test fails then the field to the right of the test name will say failed and the suggestions field will give information about how to solve the problem.

14. The following screen shot shows a test where all of the tests have succeeded.

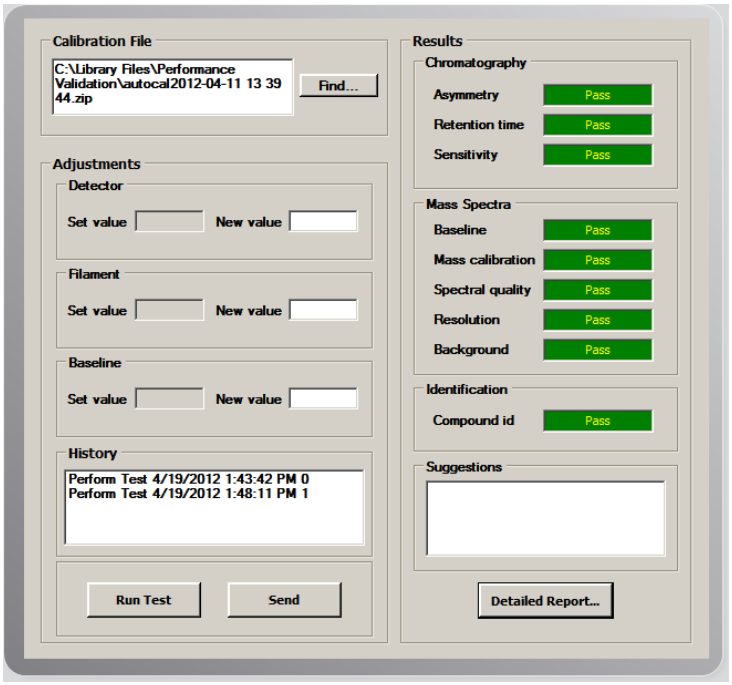


Figure 5-90 Tuning Wizard showing a system that has passed all tests

15. The following is a list of the tests and what they are testing.

Screen Results	Detailed Results	Message
Asymmetry	Asymmetry	Check Sample Amount
Retention Time	Retention Time	Check Septum and/or GC Settings or Check GC Method and/or Splits
Sensitivity	Toluene-d8 SNR TEST	No Message
Sensitivity	TIC ABSOLUTE INTENSITY TESTS	Reduce Filament 0.02 or Increase Detector Voltage -25V
Baseline	BASELINE TEST	No Message
Mass Calibration	BIN SHIFT TEST	Reduce Filament 0.02A and/or Increase Detector Voltage -25V
Mass Calibration	CALIBRATION CHECK	No Message
Spectral Quality	Bromoform 171 m/z SPACE CHARGE TEST	Reduce Filament 0.02, Increase Detector Voltage -25V
Spectral Quality	Toluene-d8 MS SPECTRAL QUALITY OVER SCANS TEST	No Message
Spectral Quality	Bromopentafluorobenzene MS SPECTRAL QUALITY TEST	Increase Detector Voltage -25V
Spectral Quality	1,2 Dibromotetrafluorobenzene 308 m/z AT APEX TEST	Increase Detector Voltage -25V
Spectral Quality	Bromoform ION STATISTICS TEST	Reduce Detector Voltage -25V
Spectral Quality	Heptane MS SPECTRAL QUALITY TEST	No Message
Resolution	Bromoform 173 m/z FWHM TEST	No Message
Resolution	1,2 Dibromotetrafluorobenzene 308 m/z FWHM TEST	No Message
Background	BACKGROUND LEVEL TEST	No Message
Compound ID	Compound ID Test	Recalibrate

16. Some of the suggestions will recommend adjusting settings on the TRIDION-9 instrument. These will be shown in the **Adjustments** field on the left side of the **Tuning Wizard** screen. The **Set value** field shows the current settings. The **New value** field shows the suggested changes.

17. The user can send the suggested changes to the instrument by clicking on the **Send** button. If the user is experienced and would like to adjust the new values before sending them to the instrument the changes can be made in the Tuning Wizard before clicking the send button.

18. The tests that return no message are for information only and are not used to tune the instrument. If a test fails but no message is displayed then the users should ignore the results and continue to run the instrument as normal.

VNC Viewer

1. The VNC (Virtual Network Computing) viewer is a utility that allows the user to see and interact with the TRIDION in real time from any PC that is connected to the instrument.

2. The instrument has been configured to work with TightVNC viewer

3. This software is free on the internet but is not supplied with the instrument.

4. To install the software Download it from the TightVNC website: http://www.tightvnc.com/download.php (Download the "Self-installing package for Windows").

5. Run the setup program. Accept all the defaults except when asked to "Choose Components". Select the "Viewer Only" on this screen. The following image shows the setup screen where the user should select the Viewer Only option.

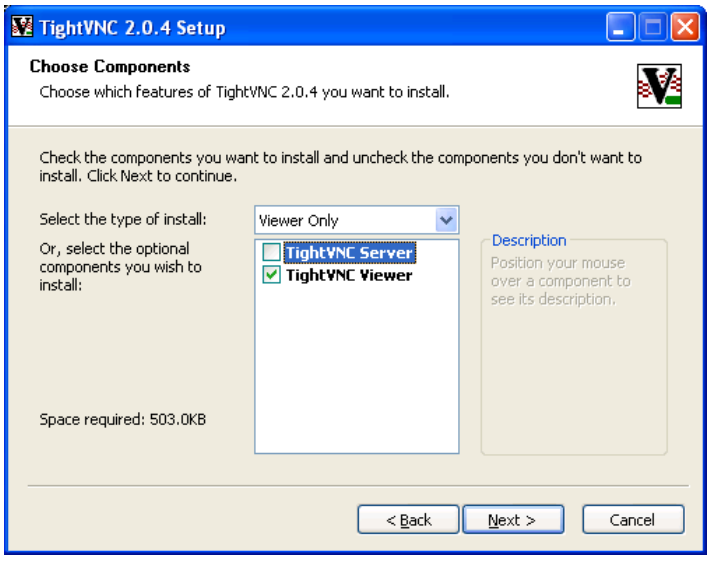


Figure 5-91 TightVNC viewer installation showing selection of Viewer Only option

6. Run TightVNC from the "Start" menu. Simply put in the IP address of the TightVNC Server (your instrument) and press "Connect". The IP address is the same one that is used in the CHROMION software to connect to an instrument. The following image shows the dialog box that opens when running the TightVNC viewer.

Figure 5-92 Dialog box that opens when running TightVNC viewer

7. An exact image of the instrument screen will appear on the computer. This image can be interacted with using the mouse and keyboard on the computer. There is a slight delay between action initiated on the computer screen and the action on the instrument.

NIST

1. The NIST software is the NIST mass spectral library as well as the AMDIS software package.

2. This is an optional software package. Any features in the CHROMION software that use the NIST data base require that the NIST software be installed.

3. To install the NIST library open the NIST folder and run the setup program, then follow the on screen instructions.

4. The NIST and AMDS are sophisticated programs. Therefore the instructions for use will not be detailed in this manual. Refer to the NIST and AMDIS documentation and help files that are included with the software for instructions on how to use the software.

Chapter 6

6 Other Operations

This chapter describes how to do other operations such as changing the battery, connecting to power, changing GC carrier gas, and other similar operations

Power supply and battery

1. The TRIDION can operate from a power supply connected to line power or a battery. Under typical operating conditions the battery will allow field operation for about 2 hours. The actual run time may vary by up to ± 15 minutes depending on the frequency of injections. The battery used in the GUARION is a 15 V 13.8 mAH rechargeable Li ion battery.

2. The battery can be charged either with an external charger or by plugging the instrument into line power while the battery is installed. When charging the battery with the instrument the instrument does not have to be on, just simply plugged into line power.

3. The following image shows the battery indicator lights on the TRIDION.

Figure 6-1 TRIDION battery indicator lights

4. If the top indicator light is lit the TRIDION is connected to line power and there is not battery installed.

5. If the second indicator light is lit then the TRIDION is operating from battery power only.

6. If the bottom indicator light is lit the TRIDION is connected to line power and the battery is installed and charging.

7. The TRIDION battery will charge when line power is connected and the instrument is not running. When the instrument is running the battery will only charge during times when the overall power draw is sufficiently low to allow extra power to be diverted to the charging operation. Power will not be drawn from the battery as long as the external line power is connected.

Changing the battery

1. Turn off the TRIDION or connect it to an external power supply (see the next section called *How to operate with external power*).

2. Lift the battery straight out of the battery compartment.

3. After removing the battery, insert the new battery into the battery compartment so the connector in the compartment aligns with the hole in the battery (see figure 4.2).

Note

Push the battery into the compartment until it is stopped by the bottom of the compartment. The battery should extend out of the compartment approximately one half inch.

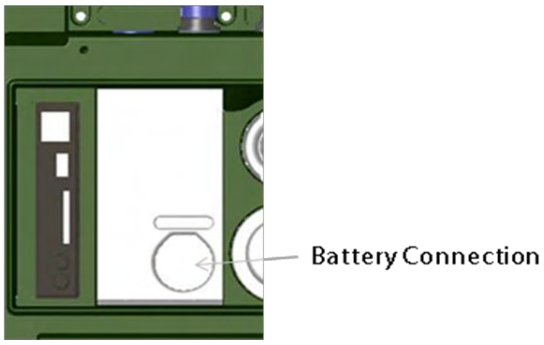


Figure 6-2 Empty battery compartment

Operating with external power

1. External power may be connected to the TRIDION at any time. The sophisticated monitoring circuitry will automatically adjust the power without interrupting the instrument performance. As described in the previous section the indicator light will change to indicate that the external power has been connected. If a battery is present then both the line power and battery power lights will be lit. The battery power will not be used when line power is connected.

2. With the correct adapters the power supply can be connected to external power from 100–250 volts 50-60 Hz AC. The following figure shows the power supply connected to the back of the instrument.

Figure 6-3 External power supply connected to the TRIDION

Changing the carrier gas cartridge

The standard helium carrier gas cartridge for the TRIDION will provide carrier gas for as many as 300 runs at 25 psi (175 kPa) operating pressure.

1. Turn the TRIDION instrument off.
2. Using the cartridge tool, remove the old helium cartridge by unscrewing it counter-clockwise.
3. Attach the new helium cartridge tightly by hand by screwing it in clockwise.

Operating with an alternate carrier gas source

1. For stationary (non-portable) operation, an alternate external carrier gas supply line can be connected to the back of the TRIDION.
2. If a helium cartridge is attached to the instrument, an external helium cylinder may also be attached to the instrument at the same time. The internal pressure of the helium cartridge is regulated to 65 ±7 PSI. As long as the external helium cylinder has a pressure of 80 PSI or greater the helium in an attached cartridge will be preserved, and can be used after disconnecting from the external helium source.
3. The external helium fitting that connects to the TRIDION is a quick connection type of fitting that attaches to 1/16" PEEK tubing.

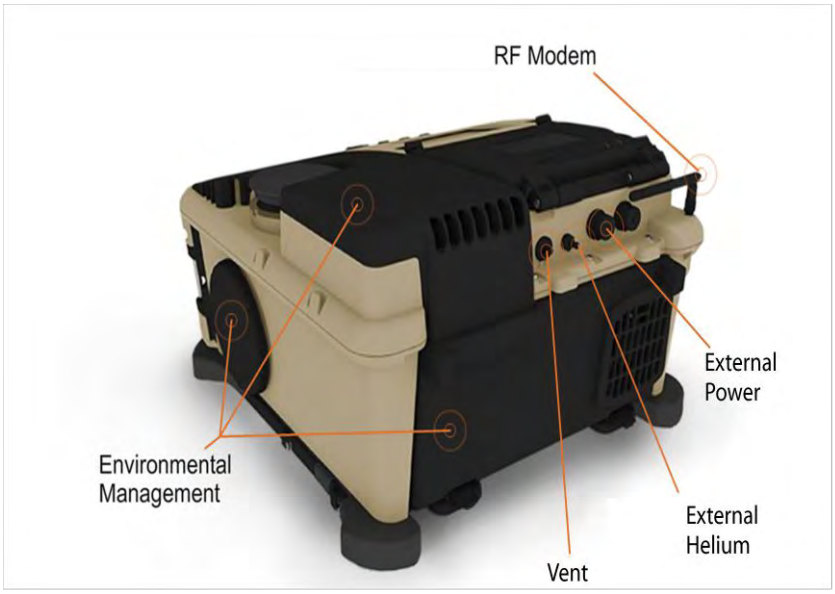


Figure 6-4 back of instrument

Caution!

Prior to the next step, regulate the external gas pressure to a minimum of 80 psi.

4. Attach the external helium carrier line by pressing the quick connect onto the helium inlet port. The quick connect is attached when it clicks into place and cannot be removed without sliding the locking cylinder back.

5. To disconnect the external helium carrier slide the locking cylinder on the quick connect back until the quick connect slides off of the instrument helium connection.

Removing/replacing the SD card

1. When removing the SD card from the TRIDION, it is best to remove the card when there is little likely hood of data being written to the card.

2. If the TRIDION is completely turned off, the SD card may be removed or inserted at any time. Otherwise the best time to remove and replace a card is when the instrument is on the Home screen.

3. Do not remove or replace the SD card when running a sample or during procedures where data or method files are being worked with.

How to "bake out" the GC injection port and column

Caution!

Baking the GC column at temperatures above 300° C may degrade the stationary phase.

Caution!

Use external power for baking the column, otherwise, the batteries will be depleted faster than during normal use.

1. Change the following parameters to 300° C: Injector Temp, Transfer Line Temp, and Column Begin Temp by using the CHROMION software to edit the instrument settings in the Gas Chromatography screen. Send and make active the modified method to the instrument.

2. Start the standard SOP and run a blank run. This will set the temperatures to the elevated setting in the modified method.

3. settings to the previous settings and again run a system blank to switch the GC parameters back to normal operating temperatures and ensure that the bake out procedure cleaned the GC properly.

Caution!

Verify that the parameters have been restored on the TRIDION by viewing the temperature settings under **Advanced** >> **Diagnostics** >> **GC**.

Chapter 7

7 Advanced Operations

This chapter explains how to use operations that are intended for expert users. These operations allow the user to adjust the way the TRIDION functions. Because the TRIDION does have a default setting, any changes will erase the previous settings. All settings should be saved on a computer before changes are made.

Accessing the Advanced screen on the TRIDION

1. The Advanced screen provides access to information about the instrument parameters and the run-time voltages and currents.

2. The primary purpose of the Advanced screen is used to troubleshoot the instrument by inspecting the voltages, currents, and other settings during sample analysis.

4. Turn on the TRIDION if it is off, otherwise begin with step **5**.

5. Select the **Advanced** button from the Home screen. The following image shows the Advanced screen.

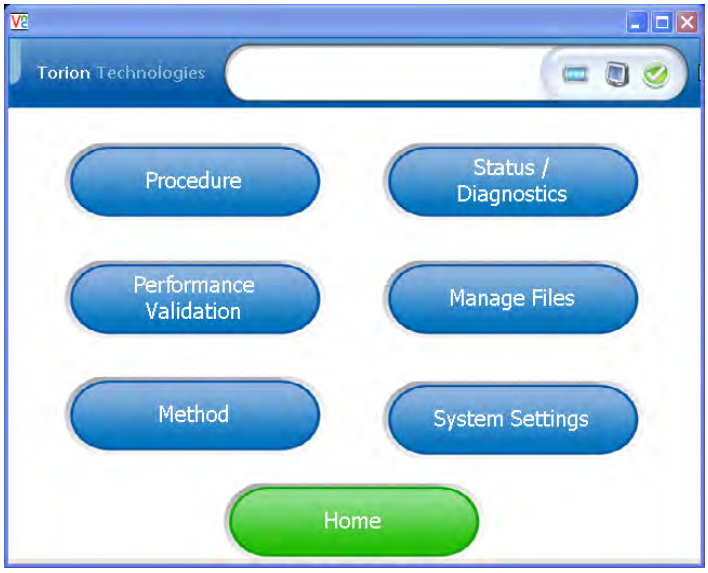


Figure 7-1 Advanced screen

6. For a complete description of all the operations available from the Advanced screen see the Advanced Screens section in the Instrument Operation chapter of this manual.

7. Exit the Advanced screen any time by selecting the **Home** button**.**

Viewing current calibration points and operating parameters

1. Current calibration points and operating parameters may be viewed in three ways: from the TRIDION instrument screen, opening the saved settings file using CHROMION software, or by retrieving the settings file from the instrument using CHROMION software.

Viewing calibration points and operating parameters on the screen of the TRIDION

1. Calibration information is found in the Status/Diagnostics section of the advanced screen.

2. Follow the instructions in the instrument control user interface chapter to access the calibration information on the instrument

Viewing calibration points and operating parameters by retrieving the method file from the instrument

1. Open the CHROMION software on a computer that is connected to a TRIDION. Follow the procedures in the software chapter to assign the correct IP address for an instrument and attach to the desired instrument.

2. From the CHROMION main screen choose the **Mass Spectrometer** section under the **Tools** tab located on the left side of the screen.

3. If an instrument is already attached to the computer the settings and calibration information will already be loaded onto the computer. If no instrument is attached then the calibration information will not be visible.

4. The settings are visible in the **MS Settings** tab.

5. Select the **MS Calibrations** tab to see the mass calibration information.

Loading operational settings onto the TRIDION

1. Methods store information about items that are affected by the chromatographic conditions. The operating settings are separate and are used to control instrument specific functions.

2. Both the method and the settings file are stored on the SD memory card. Settings become active immediately while method settings must be activated before taking affect.

3. New settings may be sent to the instrument at anytime while methods can only be sent when the instrument is not performing an analysis. If inappropriate setting changes are sent while a sample is running the analytical results will not be correct and there is a risk of locking the instrument resulting in a need to do a hard reset.

Caution!

Only voltages and temperatures can be safely changed while an instrument is performing an analysis. Other settings are used for filtering of data and may cause poor analytical results or hardware failure if changed during an analytical run.

4. Turn on the TRIDION.

5. Using CHROMION software, attach to an instrument.

6. Open the **Mass Spectrometer** screen under the **Tools** section.

7. If the instrument is attached the settings table will already be populated.

8. Adjust the setting that needs to be changed and select the send button at the top of the screen. Refer to the software chapter for details about the **Mass Spectrometer** screen.

Check or monitor the operating parameters during a run

The user may open Advanced mode and check or monitor the actual voltages, currents, temperatures, and other settings at any time.

1. Turn on the TRIDION.

2. Open the Advanced screen (see the section called Advanced screens in the Instrument Operation chapter of this manual).

3. Select the **Status/Diagnostics** button.

4. Select any of the tabs on the screen to view the parameters.

Figure 7-2 Status/Diagnostics screen sowing the Versions tab

Recommended Operating Parameters

Table 7-1 Recommended Operating Parameters

Major	Group	Name	Value	T/F	Min-Max	Unit
Control	SolventDelay	IsOn		false		
Control	SolventDelay	Value	7		None	Seconds
Control	Baseline	IsOn		true		
Control	Baseline	IsAuto		false		
Control	Baseline	Chunk	200		None	None
Control	Baseline	Value	64		30 - 75	Arbitrary
Control	Noise	IsOn		true		
Control	Noise	Threshold	1		None	Arbitrary
Control	Shot	IsOn		true		
Control	Shot	Window	1		None	Indices
Control	Shot	Threshold	0		None	Arbitrary
Control	RunningAverage	IsOn		true		
Control	RunningAverage	Window	2		None	Indices
Control	Hanning	IsOn		true		
Control	Hanning	Window	3		None	Indices
Control	Hanning	Coefficient	1.4		None	Arbitrary
Control	BinCollapse	IsOn		true		
Control	BinCollapse	Window	30		None	Indices
Control	GaussCentroid	IsOn		true		
Control	GaussCentroid	Sigma	1.3		None	Arbitrary
Control	DynamicScale	IsOn		true		
Control	NoiseRemove	IsOn		false		
Control	NoiseRemove	LowessSpan	0.1		None	Arbitrary
Control	NoiseRemove	LowessNSteps	3		None	Arbitrary
Control	NoiseRemove	IsAutoDelta		false		
Control	NoiseRemove	LowessDelta	12		None	Arbitrary
Control	NoiseRemove	CutoffWeight	1.5		None	Arbitrary
Control	NoiseRemove	CutoffThreshold	100		None	Arbitrary
Control	NoiseRemove	ShotWindow	1		None	Indices
Control	NoiseRemove	ShotThreshold	0		none	Arbitrary
GasChromatograph	Helium	Pressure Slope	0.14		.08 - .25	
GasChromatograph	Helium	StartCalibrationPressure	~18		16 – 23	
GasChromatograph	Helium	StartCalibrationTemerature	50			
MassSpectrometer	IonSource	HardSolventDelay	0			
MassSpectrometer	ionSource	FilamentCurrent	1.05		0.8 – 1.25	amps

MassSpectrometer	IonSource	FilamentBiasVoltage	-70	None	Volt
MassSpectrometer	IonSource	FilamentGateLowVoltage	-150	None	Volt
MassSpectrometer	IonSource	FilamentGateHighVoltage	150	None	Volt
MassSpectrometer	IonSource	BaseLineIsOn	true		
MassSpectrometer	IonSource	BaseLineIsAuto	false		
MassSpectrometer	IonSource	BaseLineChunk	200	None	Arbitrary
MassSpectrometer	IonSource	BaselineValue	64	30 - 75	Arbitrary
MassSpectrometer	IonSource	NumberSignificantIndexes	100	None	Indices
MassSpectrometer	IonSource	IonTarget	1000		Arbitrary
MassSpectrometer	IonSource	TargetStep	70	None	Arbitrary
MassSpectrometer	IonSource	IonizationMinimumTime	0.015	0.015-9837864	Milliseconds
MassSpectrometer	IonSource	IonizationMaximumTime	60	0.12-32	Milliseconds
MassSpectrometer	IonSource	MaximumIonizationChange Factor	100	None	None
MassSpectrometer	IonSource	MeanBound	0.63		
MassSpectrometer	IonSource	FullWidthHalfMax	0.5		
MassSpectrometer	MassAnalyzer	HardSolventDelay	0		
MassSpectrometer	MassAnalyzer	AmplitudeAVoltage	290	none	Volt
MassSpectrometer	MassAnalyzer	AmplitudeAVoltage	190	none	Volt
MassSpectrometer	MassAnalyzer	StepAVoltage	0		Volt
MassSpectrometer	MassAnalyzer	StepBVoltage	0.3		Volt
MassSpectrometer	MassAnalyzer	RampMaxVoltage	2200		
MassSpectrometer	MassAnalyzer	CoolTime	5	0.12-30.72	Milliseconds
MassSpectrometer	MassAnalyzer	ScanTime	60	0.12-32	Milliseconds
MassSpectrometer	TrapHeater	Temperature	150	125-180	Degrees C
MassSpectrometer	Detector	HighVoltageVoltage	-1775	-1250 - -2200	Volts
MassSpectrometer	Detector	HardSolventDelay	0		
MassSpectrometer	Detector	RFPhase	21	Specific for each trap	DO NOT CHANGE
MassSpectrometer	VacuumChamber	Helium.FlowRate	180	100-275	Arbitrary

Reset the on-board computer

1. There is a reset button and an emergency shutdown button on the TRIDION.

2. The reset is used to restart the CPU without turning off the system power. This is used in cases where the instrument has stopped operating and the user wants to restart the computer without losing vacuum or temperature.

3. The emergency shutdown button turns of the system power immediately. This would be used if the user notices a situation where they think the system is running away thermally or for any situation

where the user wants the system to shut down without going through the normal process. This should not be used except in emergency situations since not following the normal shut down process risks pulling contaminants from the turbo pump back into the vacuum chamber.

4. The following image shows the location of the **Reset** and **Emergency Shutdown** buttons. They are located under the utility cover on top of the instrument.

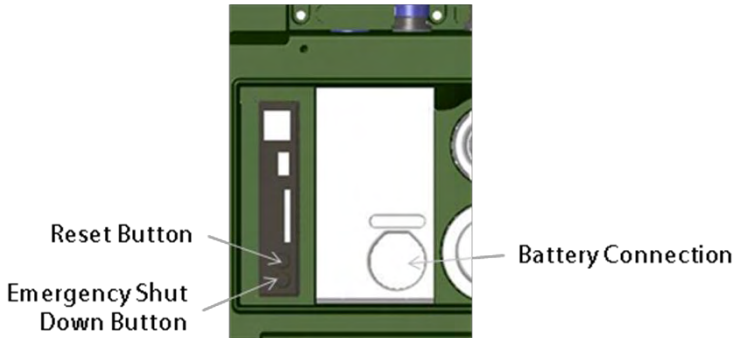


Figure 7-3 Reset and emergency shutdown buttons

5. To activate either button press it down for approximately one second and then release the button.

Delete all sample data from the SD card

1. Refer to the **Instrument Operation** chapter in the **Manage Files Section** of this manual for directions on deleting files directly from the instrument.

2. Refer to the **File Manager** section of the Software chapter of this manual for instructions on deleting and moving files from the SD card using a computer.

3. It is also possible to remove the SD card from the instrument and install it into a card reader slot on a computer. The use standard Windows functionality to view, move or delete files from the card.

TRIDION Manual Mass Calibration

1. Preparations

    a. Chemicals used in calibrating a TRIDION instrument.

        i. Provided standard CALION Performance Validation calibration vial (CV) mix.

        ii. The image below shows a chromatogram of the Performance Validation mix.

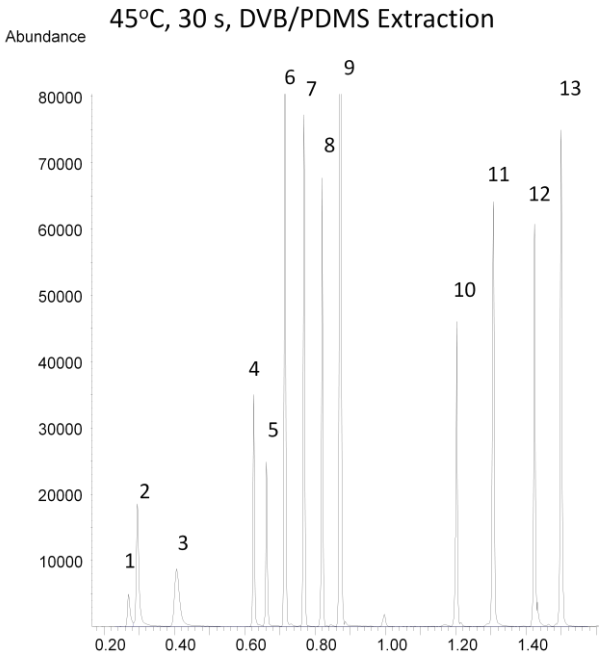


Figure 7-4 Chromatogram of the CALION Performance Validation mix

iii. The CALION mix contains the following 13 compounds. The order of the list matches the elution order shown in the above chromatogram.

Compound	µL/g
1. Acetone	1.5
2. Methylene chloride	1.5
3. Methyl-tert-butyl ether	2.2
4. Heptane	1.5
5. Methylcyclohexane	0.7
6. Toluene-d8	0.7
7. Perchloroethylene	0.7
8. Bromopentafluorobenzene	0.7
9. Bromoform	0.7
10.1,2-Dibromotetrafluorobenzene	3.0
11. Methylsalicylate	6.0
12. Tetrabromoethane	6.0
13. Tetradecane	74.6

2. Steps

    a. Set GC Settings.

        i. Set column temperature settings in CHROMION/Settings/GC as follows:

Column Begin Temperature (°C):	50
Column Final Temperature (°C):	270
Column Ramp Rate (°C/sec):	2.0
Column Begin Temp Hold Time (sec):	10
Column Final Temp Hold Time (sec):	20

    b. The instrument must be in uncalibrated mode.

        i. Uncalibrated data shows the bins of data used to create mass spectra. The TRIDION electronics stores the data from an analysis in 4096 discrete locations or bins. The mass range of the instrument is 500 amu. The number of bins per mass is obtained by dividing the number of bins by the mass range of the instrument. So there are about 8 bins per 1 amu. In order for the instrument to display correct mass information it is necessary to calibrate which bin corresponds to which mass. The difference from instrument to instrument is usually only a few bins but this can be enough to shift the mass assignment and result in poor peak identification.

        ii. The following image shows three masses from bromoform. The masses are 171, 173, and 175. When calibrating the bin number at the apex of the bin distribution is used to correlate the bin to the specified mass. So mass 171 correlates to bin 1,157 and mass 173 correlates to bin 1,175.

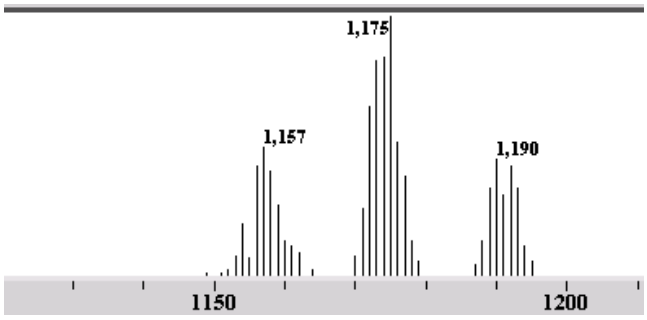


Figure 7-5 Uncalibrated bin data for bromoform masses 171, 173, and 175

        iii. The following image shows the same sample with the collapsed bins and properly assigned masses.

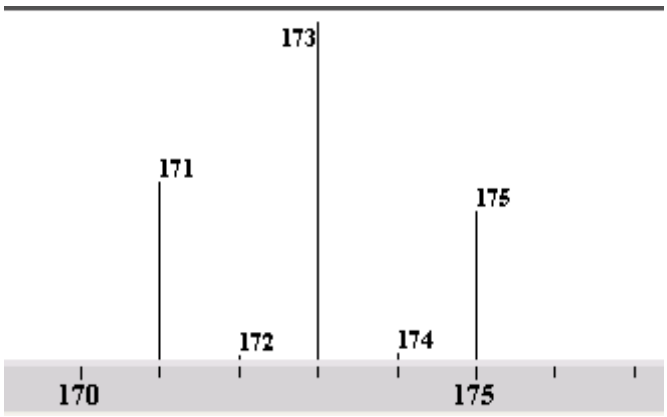


Figure 7-6 Calibrated mass data for bromoform masses 171, 173, and 175

iv. The following procedure changes the instrument settings to produce uncalibrated data from the TRIDION.

v. In CHROMION **Mass Spectrometer** screen select the **MS Calibrations**, and uncheck the **Use auto-calibration data** and if checked uncheck the **Manual** check box.

vi. In CHROMION **Mass Spectrometer** screen **MS Settings** tab , change the following values.

Control/RunningAverage/IsOn/false

Control/Hanning/IsOn/false

Control/BinCollapse/IsOn/false

Control/GaussCentroid/IsOn/false

vii. Select the **Send Mass Spec Settings to Instrument** button.

viii. The instrument will return a message saying that the method was successfully sent.

c. Set mass calibration.

i. Refer to the Software chapter section on the **Performance Validation** screen for details about setting up the mass and retention time calibration information.

ii. Run a sample from the CALION vial by placing the SPME fiber into the vial following the procedures described in the How to sample headspace vapors from liquid or solid samples section of the Basic Operations chapter.

iii. Follow the standard procedure for starting a run by running the SOP and follow the instructions to inject the CALION standard into the instrument.

iv. After the analysis use the **File Manager** to move the .RES file over to the computer. Refer to the Software chapter for details about using **File Manager**.

v. Use CHROMION **Data Review** to open the file. Refer to the Software chapter for details about the functionality of **Data Review**.

vi. The TIC should look like the example chromatogram shown above.

vii. Position the cursor over the methylene chloride peak. This should be the second peak and should elute at around 17 seconds.

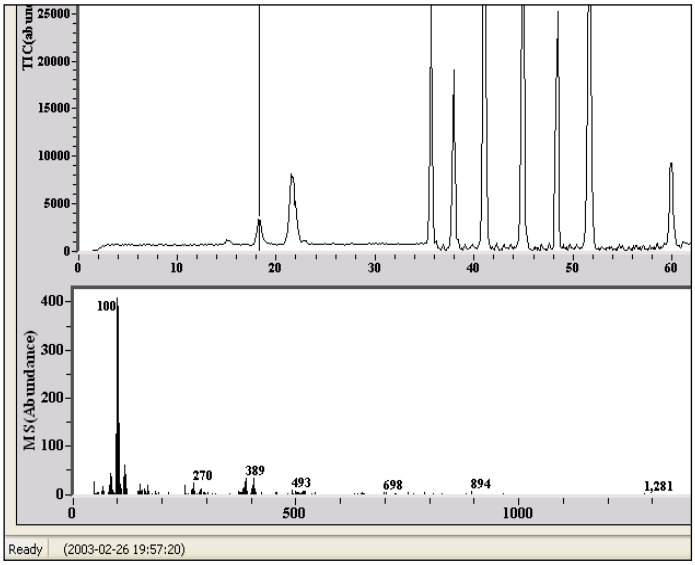


Figure 7-7 Uncalibrated mass spectral data of methylene chloride used for calibration

viii. In the example shown above the bin number for methylene chloride is 100. Open the Performance Validation screen in the CHROMION software and select Methylene Chloride from the table. The following shows that the Methylene Chloride mass is in the mass window. If the mass is not in the window adjust the minimum and or maximum values so that it is in the window.

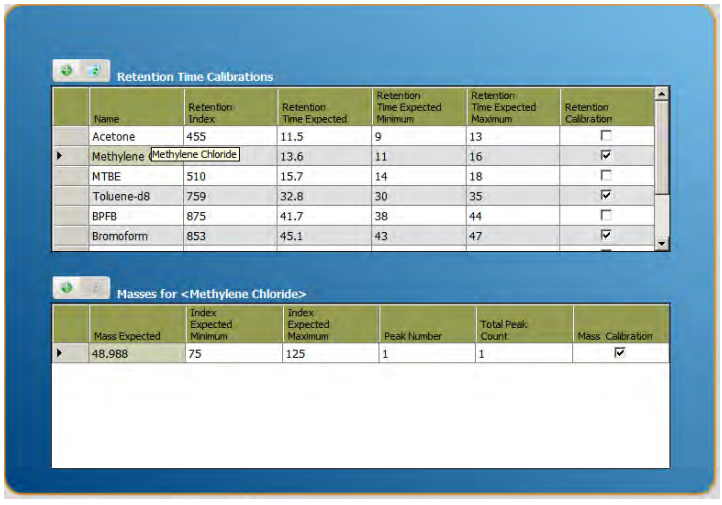


Figure 7-8 Methylene Chloride mass calibration in Performance Validation screen

ix. When using manual calibration the mass and bin number are entered into the manual calibration data section of the MS Calibrations in the Mass Spectrometer window.

x. The next mass is from the MTBE peak. Return to the Data Review screen. The following image shows the TIC with the cursor on the MTBE peak.

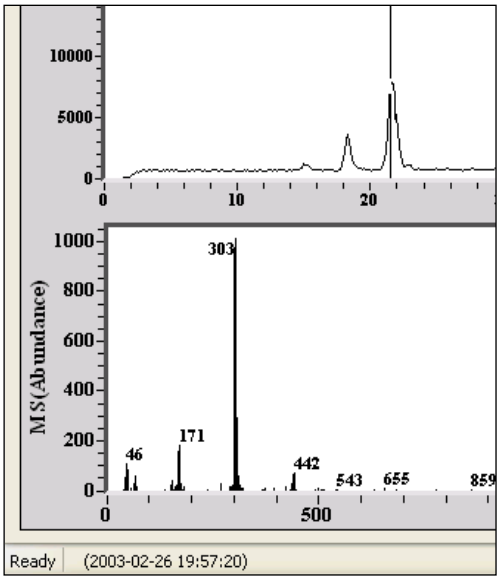


Figure 7-9 Uncalibrated mass data for MTBE

xi. The actual bin number for the 73.065 mass is 303. Return to the **Performance Validation** screen and select MTBE from the table to verify that the mass is in the window. If the mass is not in the window adjust the minimum and or maximum values so that it is in the window to adjust the settings that will be used for auto calibration. For manual calibration return to the **MS Calibration** tab in the **Mass Spectrometer** screen and enter in the mass and the bin number in the manual calibration data table.

xii. Continue this process for each of the compounds that are used for calibration.

xiii. The following table shows the chemicals that are typically used for calibration and the masses associated with the compound. The bromopentafluorobenzene (BPFB) has two masses that are used.

Chemical	Mass
Methylene Chloride	48.988
MTBE	73.065
BPFB	116.995
Methyl Salicylate	152.047
Bromoform	172.908
BPFB	247.908
Dibromotetrafluorobenzene	307.828

xiv. In some cases it may be necessary to zoom in the view of the uncalibrated mass data to accurately determine the correct bin number for a given mass.

xv. The following image shows the zoomed in uncalibrated spectral data for bromoform. The masses are 171, 173, and 175.

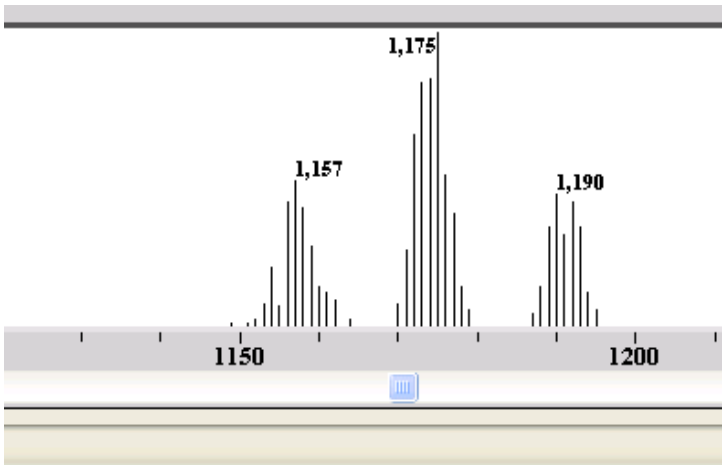


Figure 7-10 Uncalibrated bin data for bromoform masses 171, 173, and 175

xvi. After all of the data for the masses and corresponding bin numbers have been entered it is necessary to return the TRIDION to the proper settings so that the new mass calibration will be used.

xvii. To use manual calibration leave the **Use auto-calibration data** box unchecked.

xviii. Place a check box in the **Manual** check box.

xix. In CHROMION Mass Spectrometer screen change the following values.

Control/RunningAverage/IsOn/true

Control/Hanning/IsOn/true

Control/BinCollapse/IsOn/true

Control/GaussCentroid/IsOn/true

xx. Send the new settings to the TRIDION by selecting the **Send Mass Spec Settings to Instrument** button on the menu bar.

d. Validate the calibration using the CALION mix.

i. Run a sample from the CALION vial by placing the SPME fiber into the vial following the procedures described in the How to sample headspace vapors from liquid or solid samples section of the Basic Operations chapter.

ii. Follow the standard procedure for starting a run by starting the SOP and following the on screen instructions to inject the CALION standard into the instrument.

iii. After the analysis use **File Manager** to move the .RES file over to the computer. Refer to the Software chapter for details about using **File Manager**.

iv. Use CHROMION **Data Review** to open the file. Refer to the Software chapter for details about the functionality of CHROMION **Data Review**.

v. Evaluate the masses look at each scan in the peaks rather than the average. At least 80% of the scans for each peak should have the correct masses. The

following list contains all the peaks in the CALION mix along with a few of the masses in each compound. The data file should have all of the listed masses correctly identified to validate the calibration.

Compound	Masses
1. Acetone	42, 59
2. Methylene chloride	49
3. Methyl-tert-butyl ether	57, 73
4. Heptane	56, 57 70, 71
5. Methylcyclohexane	55, 83
6. Toluene-d8	98, 100
7. Perchloroethylene	129, 164, 166, 168
8. Bromopentafluorobenzene	117, 246, 248
9. Bromoform	171, 173, 175
10.1,2-Dibromotetrafluorobenzene	79, 98, 117, 148, 306, 308, 310
11. Methylsalicylate	92, 120, 121, 152
12. Tetrabromoethane	81, 107, 186, 263, 265, 267
13. Tetradecane	71, 85

vi. If each mass does not match the list above, then the instrument needs to be recalibrated.

vii. To recalibrate repeat above procedure.

TRIDION Auto Calibration (Performance Validation)

1. Open the Advanced screen on the TRIDION.
2. Select the Procedure button and end the procedure.
3. Use the **Home** button then select the **Advanced** button to return to the **Advanced** screen.
4. Select the **Performance Validation** button and follow the on screen instructions.
5. Run the 13-mix CALION standard.

6. The instrument should give the following report.

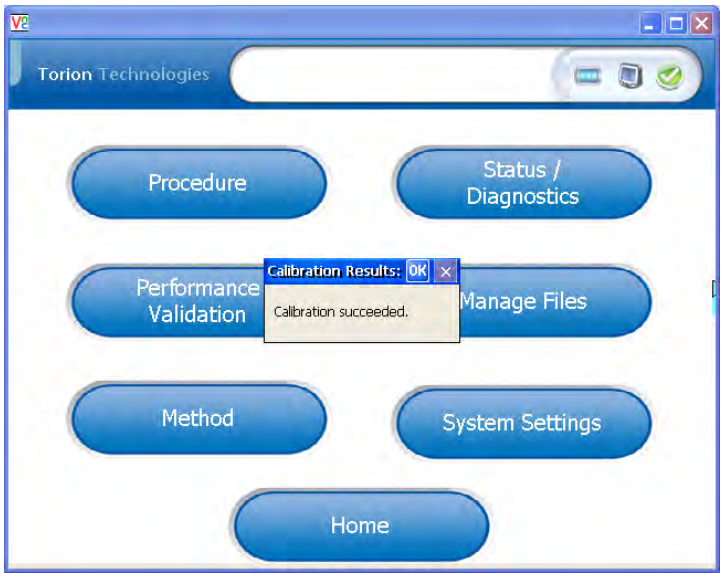


Figure 7-11 Calibration succeeded

7. If the calibration succeeded then press the **OK** button and then press the **Advanced** button and select **Procedure** and reactivate the SOP. For detailed instructions on running samples refer to the Instrument Operation chapter.

Confirm auto calibration (Performance Validation)

1. To confirm that the calibration is working follow the steps in the SOP until you can run a normal standard and run the CALION standard again. Make sure that all 13 compounds in the standard are successfully identified by the TRIDION. If all of the compounds are properly identified then the instrument is calibrated and ready to run analysis.

2. In a few cases even after running auto calibration the instrument may fail to properly identify all of the compounds in the CALION standard. If this occurs continue to the next section and follow the instruction about how to correct a failed auto calibration.

Correcting failed auto calibration (Performance Validation)

1. If the following report is displayed then the calibration failed and the calibration .ict files needs to be modified to adjust the ranges around the various masses and retention times being used for calibration.

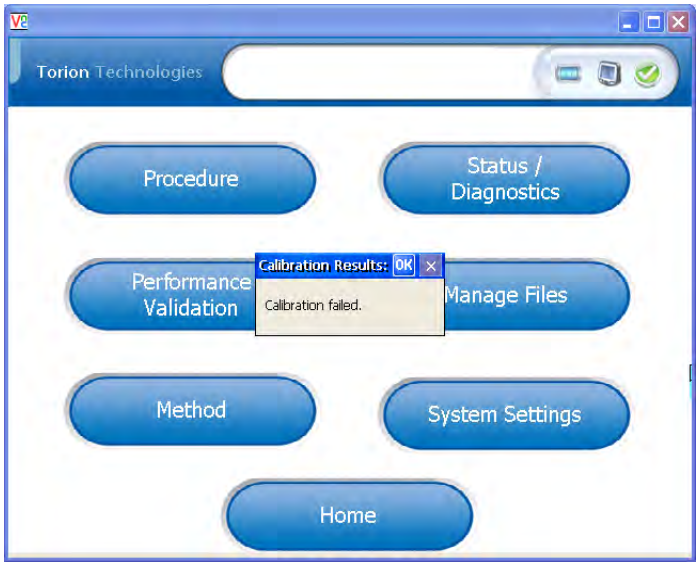


Figure 7-12 Auto calibration failed message

2. If the calibration fails connect the instrument to a computer.

3. Open the CHROMION software.

4. Follow the instructions in the CHROMION software section of this manual for instructions on how to connect the computer to the TRIDION.

5. Open the **Performance Validation** section of the CHROMION software.

6. The following image shows the window that will open after selecting the **Performance Validation** option.

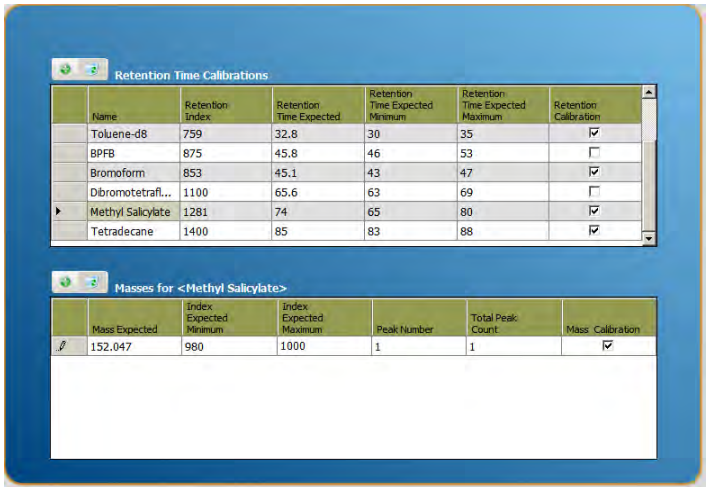


Figure 7-113 CHROMION Performance Validation screen

7. The windows for retention time and mass calibration are shown in the **Performance Validation** tables. The retention times are in the top table and the masses are in the bottom table. To select a compound click on the compound name in the top table and the mass data displayed in the bottom table will change to the data associated with the selected compound.

8. Most of the time an auto calibration fails because one of the retention times or mass calibration bins has changed and is no longer in the window set in the method. To check the information it is necessary to open the last auto calibration data file.

9. Use the **File Manager** to browse to the storage card/calibration/data folder on the storage card. Move the file to a location on the PC and then use CHROMION **Data Review** to open the file. The file will look different because it is collected with unusual system settings and contains uncalibrated data. The system needs to run this way in order to create a calibration file correctly.

10. In the following image the cursor has been placed on the methyl salicylate peak.

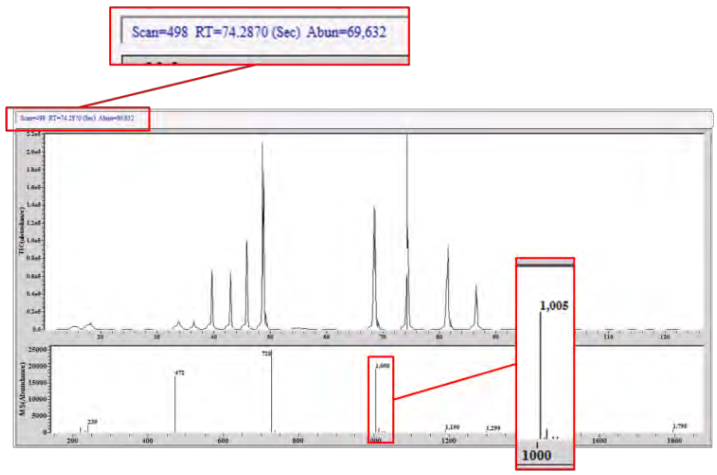


Figure 7-124 Performance Validation correction showing methyl salicylate peak with binned, centroided but uncalibrated data

11. Just below the button row in the upper left corner of the screen there is a numerical listing of the cursor position. This includes the scan number, retention time and abundance for the selected scan.

12. The retention time (RT=74.287) rounds to 74.3 seconds. The table shows the retention time window as low 65 high 80 and ideal 74. So the actual peak falls within the specified retention time window and would not cause the calibration to fail.

13. Place the cursor on each peak and verify that the retention time is within the defined retention time window for the peak.

14. The following image shows the cursor placed on the bromopentafluorobenzene peak.

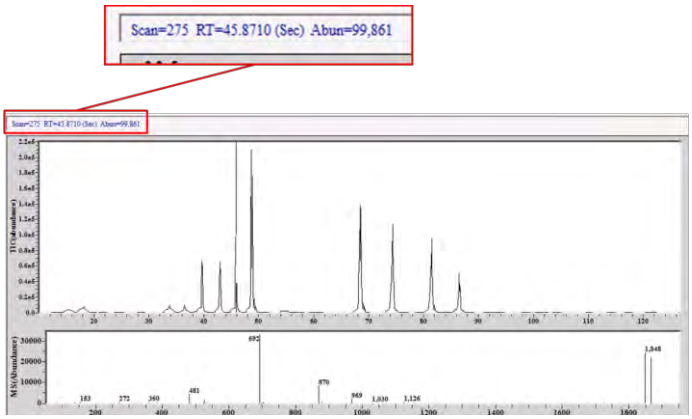


Figure 7-135 Performance Validation correction showing bromopentafluorobenzene (BPFB) peak with binned, centroided but uncalibrated data

15. According to the **Performance Validation** table the BPFB peak retention time should be 48.1 and it has a window from a low of 46 to a high of 53. The actual retention time of the BPFB peak is 45.8. This is not within the retention window set in the calibration table. As a result the calibration will fail. To fix this change the calibration window to a low of 42 and a high of 50 with an ideal time of 45.8.

16. The same process must be completed for all peaks used in the auto calibration file to determine that the actual retention times are falling within the set retention times.

17. The same process must be completed for mass calibration.

18. The following shows the methyl salicylate peak highlighted. The mass that is being used for calibration is mass 152.047. This corresponds to a bin number of 1005.

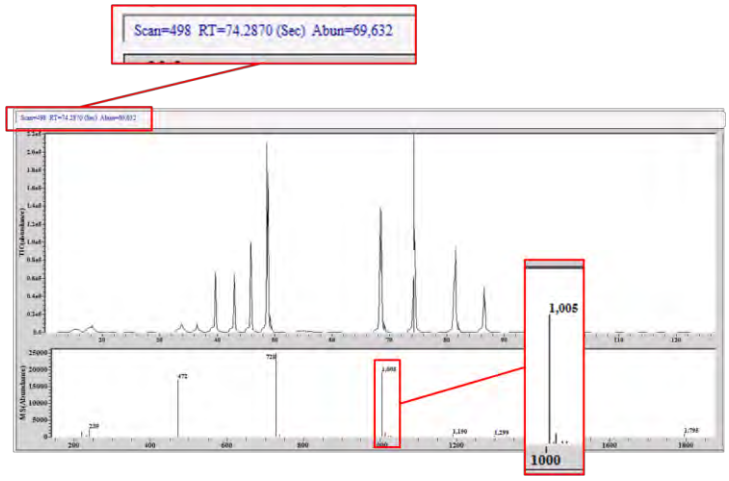


Figure 7-146 Performance Validation correction showing methyl salicylate peak with binned, centroided but uncalibrated data

19. The Mass Calibration table above has a window of 980 to 1000. As a result the methyl salicylate peak will fail calibration since the actual index is 1,005 as shown in the figure above. To fix the mass calibration change the window so it is more centered on the actual bin number of 1005 by setting the low index to 995 and the high index to 1015.Repeat this process for each of the peaks and the associated masses. Once all of the data has been corrected save the method and then send the new method to the instrument by selecting the **Send Method to Instrument** button.

Chapter 8

8 Service

This chapter describes how to perform certain service operations on the TRIDION.

Trap service tools and materials

1. The following table contains a listing of the tools provide in the instrument tool bag. Not all of these tools provided are used for cleaning the trap but all of the tools needed are part of the tool kit.

Table 9-1 Tool list and descriptions

Part Number	Tool Description
4340-0058	Gauge DOWEL PIN, 0.0580" OD X 2" L, SST (EGUN alignment tool)
6420-0056	5/64"Hex driver (#2) [for trap screws]
6420-0060	Flat head screwdriver 0.078" wide blade [RF tuning]
6420-0064	3/32" Hex driver (#4) [GC screws]
6420-0068	7/64" x 50 hex driver (#6) [Vacuum cap screws]
6420-0080	3/16 open end wrench(#4 nuts)[for trap electr. standoffs]
6420-0081	1/8" nut driver (#0) nut) [for filament nuts]
6420-0094	1/4" and 5/16" open end wrench [for PEEK tubing nuts]
6420-0095	5/32" nut driver (#2) [for EGUN nuts]
6420-0096	T10 TORX® driver 3/16" blade diameter [for white RF board cover]
6450-0018	Tweezers, #7, Curve [Filament C-clip]

2. The materials, tools, and working surface should be thoroughly cleaned to remove any contaminants. Any user that will be handling any parts internal to the vacuum chamber needs to be wearing lint free laboratory gloves.

O-ring Handling, Cleaning, Installation, and Removal

1. Tools and Supplies

    a. Dust-off
    b. Lint-free tissue - Kimwipes

c. Clean lint free antistatic gloves or very clean hands
d. Tool for removing o-rings that will not scratch the surface of the o-ring groove – wooden or plastic tooth pick or plastic tweezers
e. Cleaning solvent- technical grade or better methanol or ethanol
f. Loop or magnifying lens

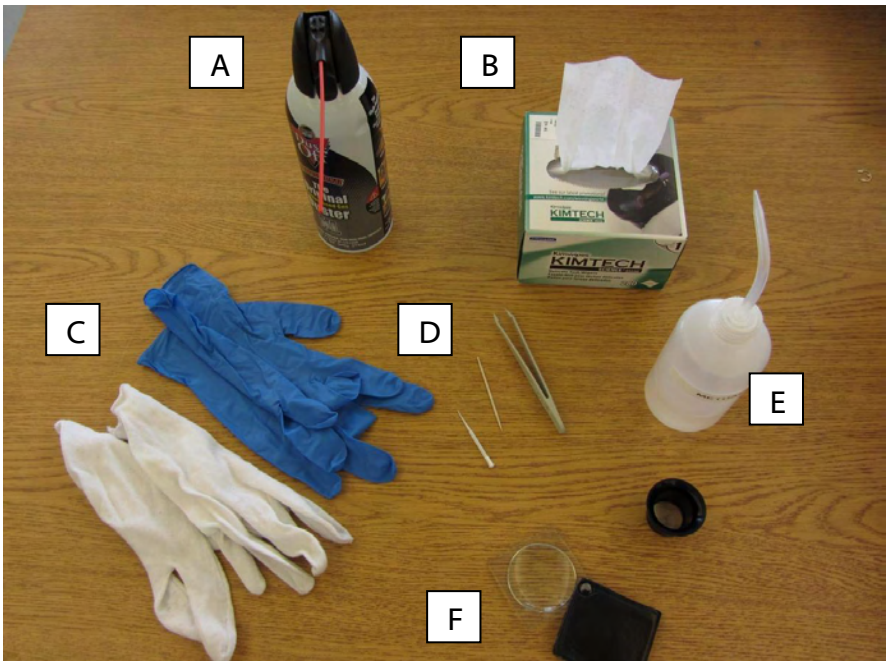


Figure 8-1 Dust off(A), Kimwipes(B), Lint-free antistatic gloves(C), Tool for removing o-rings that will not scratch the surface of the o-ring groove(D), Methanol(E), Magnifying lens(F)

Removing o-rings:

1. Sharp hard or metal tools should never be used to remove o-rings. Use plastic or wooden tools as shown in Figure 1D. Proper removal of o-ring is illustrated in the following figure.

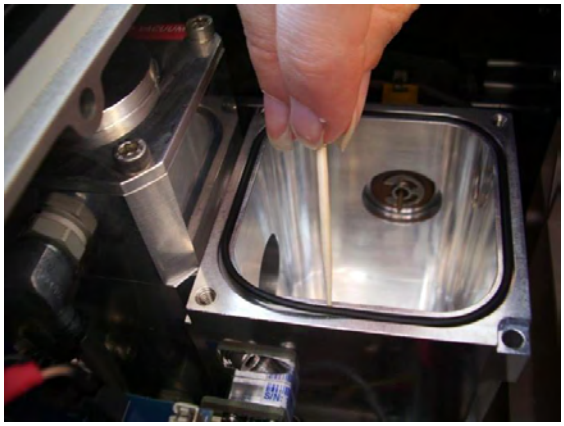


Figure 8-2 Proper removal of o-ring

Installing o-rings:

2. Before handling any parts or o-rings wash clean antistatic gloved hands or bare hands with soap and deionized water. Do not use plastic or elastomeric gloves that are not antistatic (they attract dust). Make sure you rinse several times and ensure all soap is removed from gloves or hands. If you use lint-free cotton gloves make sure they are really lint free, not over used, and clean.

3. Clean o-ring groove with lint-free tissue and cleaning solvent. The best way to do this is to wet the tissue with the solvent and wipe the o-ring groove, ensuring that the wipe directly contacts the sealing surfaces of the groove. The following image shows how to do this.

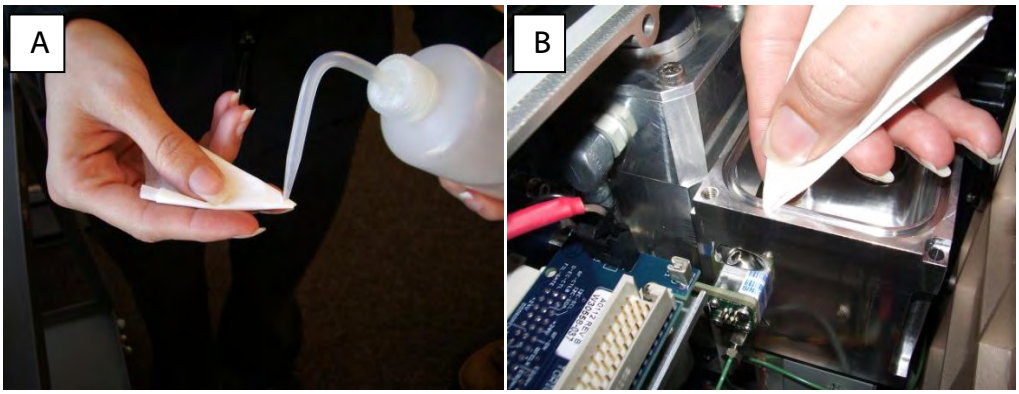


Figure 8-3 Wet lint free tissue with cleaning solvent (A) Clean o-ring groove with wet tissue (B)

4. Clean mating surface to the o-ring with lint free tissue and cleaning solvent. The best way to do this is to wet the tissue with the solvent and wipe the o-ring mating surface. The following image shows how to do this.

Caution!

When handling all components (e.g., ion trap module) do not touch areas of the components in locations that reside directly in the high-vacuum chamber when assembled.

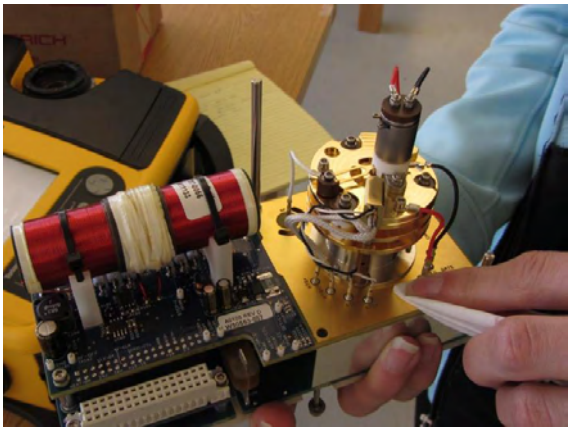


Figure 8-4 Cleaning o-ring mating surface

5. Use dust-off to remove any particles from the groove and surface. The following image shows how to do this.

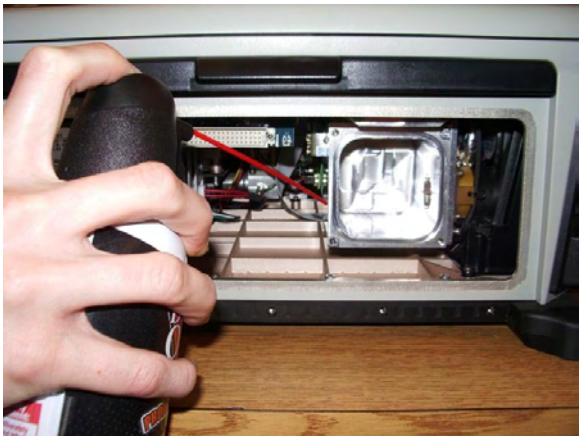


Figure 8-5 Dust-off o-ring groove

6. Inspect groove and surface for attached particle and dirt. If there are any particles or dirt attached to the o-ring groove or mating surface clean again (steps 1-3).

7. Inspect o-ring carefully to make sure that there are no cracks, dimples, cuts, abrasions, embedded particles or excessive flash. The following image shows how to do this. It is recommended to start with a new o-ring as opposed to re-cleaning a previously used o-ring.

Figure 8-6 Inspecting o-ring for defects

For round cross section o-rings make sure there are not any flat or obround sections. For square or quad cross sectioned o-rings make sure they have a consistent thickness in both directions.

8. Clean o-ring with lint-free tissue and cleaning solvent. The best way to do this is to wet the tissue with the solvent and wipe the o-ring. The following image shows how to do this.

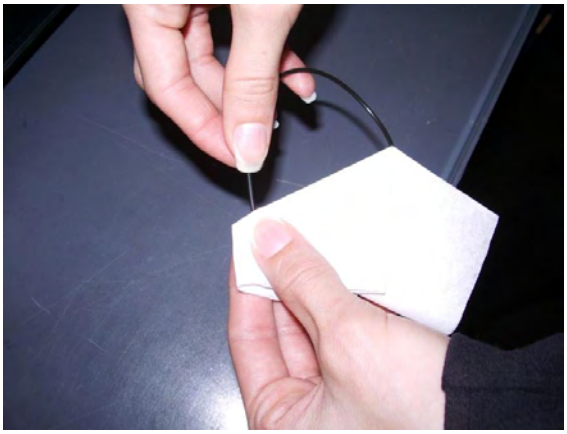


Figure 8-7 solvent Cleaning the o-ring with solvent wetted lint-free tissue

9. After solvent cleaning the o-ring use dust off to remove any remaining particles and inspect o-ring to ensure that it is clean (refer to the figure in step 6). The following figure shows how to use the dust-off to clean the o-ring.

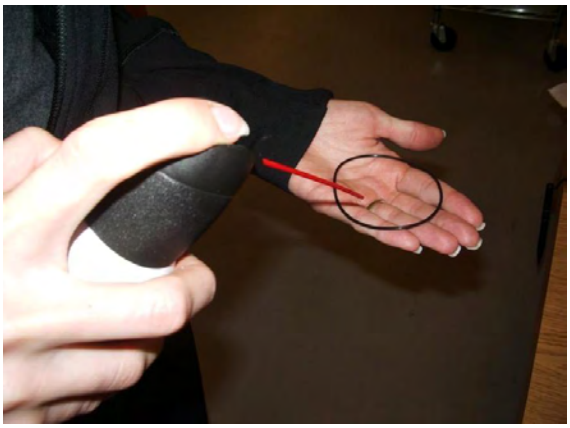


Figure 8-8 Using dust-off to remove dust particles from an o-ring

If the o-ring is not clean repeat the cleaning process (steps 7 and 8).

Caution!

Do not lay the o-ring down on a surface that is not clean and dust free. If you need to put the o-ring down it is recommended that you lay it on a clean lint free tissue. See the following figure.

Figure 8-9 Storing a clean o-ring in a dust free environment

10. Carefully lay the o-ring into the o-ring groove. The following image shows how to do this.

Figure 8-10 Placing o-ring into vacuum chamber groove

Be careful to not roll the o-ring into the groove. It is important the tool parting lines on the o-ring are facing the groove sides.

O-rings tolerances are designed so that they may possibly have a slight interference with the inside edge of the o-ring groove so you may need to gently stretch the o-ring a very small amount in order to get it to lay flat. Be very careful to not over stretch the o-ring. The following image shows the effect of o-ring groove tolerances on o-ring installation.

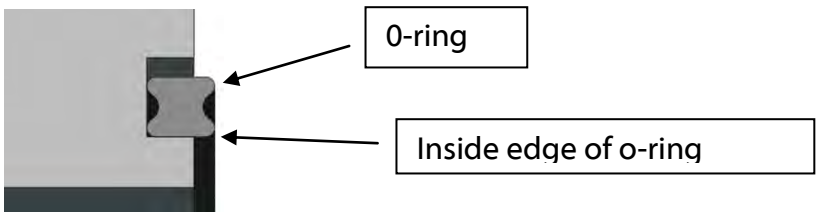


Figure 8-11 Effect of o-ring groove tolerances on o-ring installation

Once the o-ring is in place inspect the o-ring, o-ring grove and mating surface for dust and dirt. Use the dust-off to remove any particles. The following figure shows the use of dust-off to remove dust particles from the installed o-ring and the mating surface.

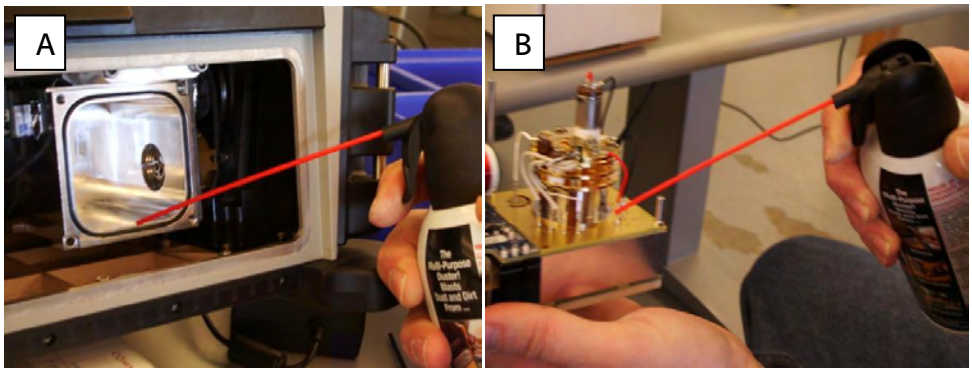


Figure 8-12 Use of dust-off to remove dust particles from the installed o-ring and the mating surface

11. Assemble the mating surface to the o-ring and the groove and uniformly tighten screws.

Remove the ion trap/RF module

1. Use the 7/64" hex driver to remove the front cover of the TRIDION. There are 5 screws along the bottom edge of the cover. After the screws have been removed pull the bottom of the cover. As the cover pulls forward the top edge must drop down to remove the cover. Set the cover aside. The following image shows an expanded view with the front cover removed.

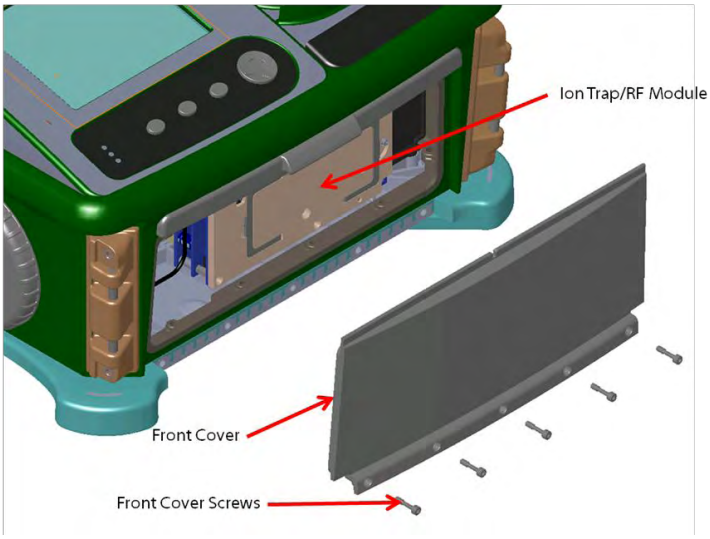


Figure 8-13 TRIDION front cover removal

2. Using the same 7/64" hex driver loosen the two captive screws that are holding in the ion trap/RF module. Use the handles to pull the ion trap/RF module out of the TRIDION. The following image shows the ion trap/RF module removed from the TRIDION.

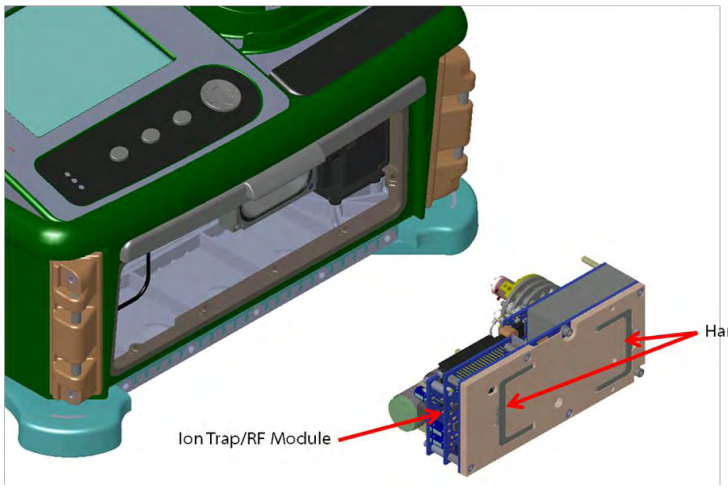


Figure 8-14 Ion trap/RF module removal

Trap maintenance procedures

Trap disassembly

1. The following image shows an expanded view from the trap side of the ion trap/RF module. The following instructions will tell how to disassemble the trap portion of the module. Use this image as a reference during the disassembly of the module.

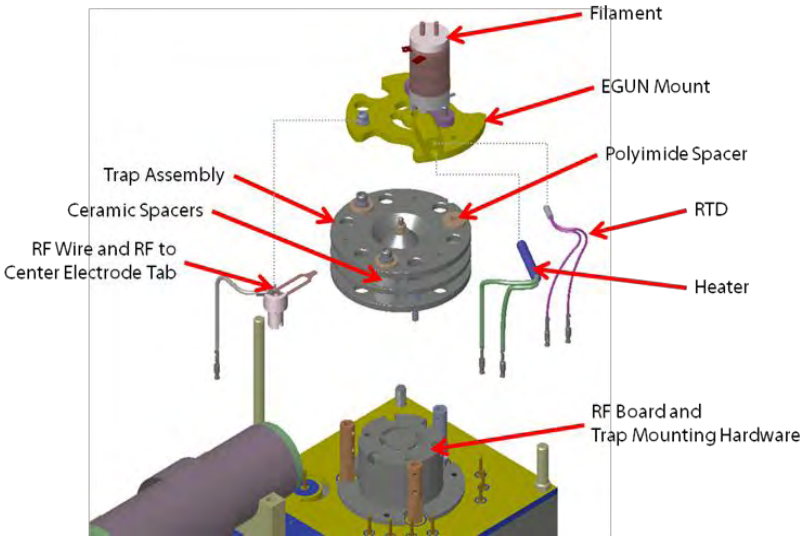


Figure 8-15 Exploded view of main trap components

2. The following image shows the location of the wires on the trap assembly.

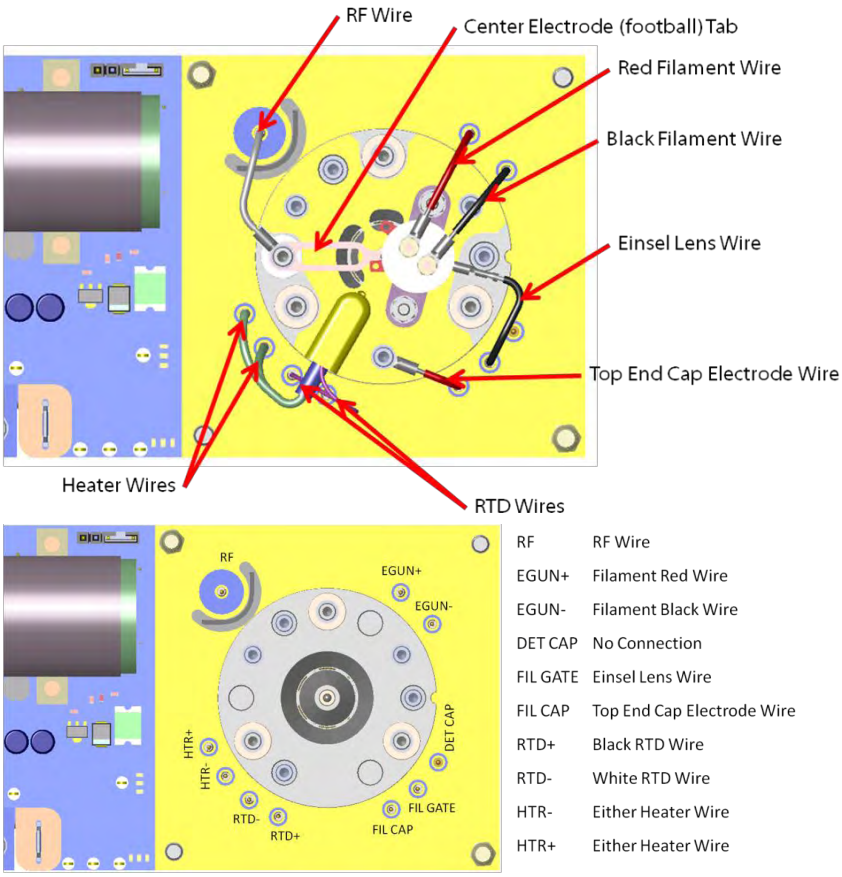


Figure 8-16 Trap wire locations

3. Gently pull the wires for the Heater, RF, Red and Black Filament wires, Einsel Lens, Top End Cap Electrode and RTD loose from the pins on the board.

4. The 5/64" hex driver is used for all of the screws on the trap assembly.

5. Remove the screw that is holding the RF wire and RF tab to the center electrode (football). Remove the wire, tab and spacer and set them aside on a clean dust free surface.

6. Remove the screws that are holding the EGUN mount onto the top of the trap assembly. Lift the EGUN mount off of the trap assembly and set it aside on a clean dust free surface.

7. Remove the screws that are holding the trap assembly onto the RF board assembly and lift the trap off of the board assembly. Set the board assembly aside on a clean dust free surface.

8. The trap assembly has many ceramic spacers that are used for electrical isolation and alignment of the parts. Make sure that you are working over a flat surface that is clean and dust free. Place the trap on the clean dust free surface and carefully remove the screws that are holding the trap assembly together. The ceramic spacers may fall out as the screws are being removed this is normal just make sure they all stay together and stay clean.

Trap cleaning procedure

1. The cleaning is done by placing the two end cap electrodes, the ring electrode and the center electrode (football) in 35% hydrogen peroxide and heating it enough to where the solution boils. Allow the parts to soak in the boiling solution for 30 minutes. Be careful to avoid scratching or in

other ways damaging the curved surfaces of the electrodes and end caps. Damaged parts must be replaced for proper performance of the instrument.

Caution!

The gold plating is thin. Use of brushes or other abrasive cleaning materials will remove the plating and cause permanent damage to the performance of the trap.

2. Carefully remove the electrodes from the peroxide solution and place them in a clean beaker of deionized water. This will ensure that the peroxide solution and any contaminants that were removed from the trap parts do not redeposit before being rinsed off by the deionized water.

3. Further rinse the parts thoroughly with more deionized water and allow them to fully dry before reassembly.

Trap reassembly

1. The following image shows the electrodes.

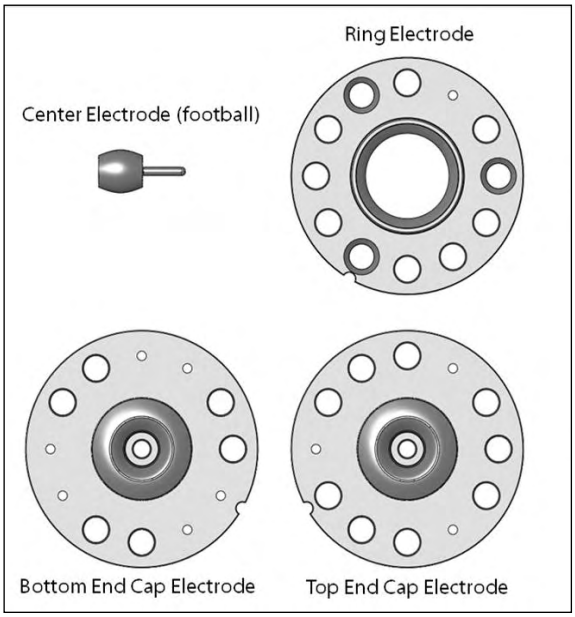


Figure 8-17 Trap electrodes

2. Use the alignment fixture to reassemble the trap.

3. Install the alignment pins in the Bottom End Cap electrode. The Bottom End Cap Electrode is differentiated from the Top End Cap Electrode by the number of larger holes. The Bottom End Cap Electrode has fewer larger holes than the Top End Cap Electrode refer to the last image for help in properly identifying the electrodes.

4. Place the Bottom End Cap Electrode on a clean flat surface with the curved side up. Refer to the previous image for help in identifying which electrode is the Bottom End Cap Electrode. The first pin is installed in the first threaded hole clockwise from the notch. The image below shows the Bottom End Cap Electrode with the alignment pins in place.

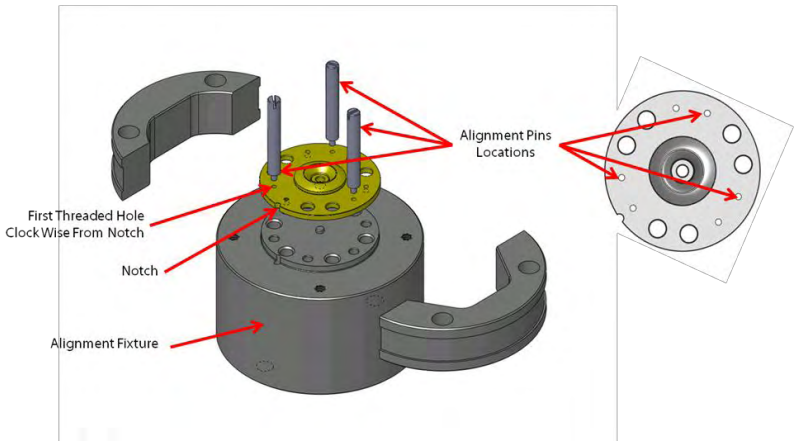


Figure 8-18 Alignment pin installation

5. Leave the alignment pins loose so they can move during assembly. The correct installation would be to tighten them until they stop then turn them back 1/4 turn.

6. Place the Bottom End Cap Electrode and alignment pins into the Alignment Fixture. Make sure the notch on the Bottom End Cap Electrode aligns with the notch in the Alignment Fixture.

7. Slide three of the ceramic spacers over the alignment pins.

8. Place the bottom polyimide spacer for the center electrode (football) in the center of the Bottom End Cap Electrode. The polyimide spacer is symmetrical so it does not matter which side is up.

9. Place the Center Electrode (football) onto the polyimide spacer.

10. The next part to install is the Center Ring Electrode. Look at the larger holes in the electrode. One side of the holes has a bevel and the other side is flat. Slide the Center Ring Electrode over the alignment pins with the beveled side down. Make sure the notch aligns with the notch in the alignment fixture and the Bottom End Cap Electrode.

11. Place the top polyimide spacer on the stem of the Center Electrode (football). Make sure the taller part of the spacer is up.

12. Slide three more of the ceramic spacers onto the alignment pins.

13. Slide the Top End Cap Electrode onto the alignment pins with the curved surface down. Make sure the notch aligns with the notches in the Alignment Fixture, Bottom End Cap Electrode and Center Ring Electrode.

14. Remove one of the three alignment pins.

15. Install one of the three screws with the polyimide spacer in the hole where the alignment pin was removed and tighten it so it just begins to clamp the assembly together. In a later step the rings still need to be able to move so do not over tighten the screw at this point.

16. One at a time remove each of the other alignment pins and replace them with the screws and polyimide spacers. Tighten them so they just begin to clamp the assembly.

17. Grasp the outside of the Alignment Fixture and gently squeeze so that the inside comes in contact with the trap assembly on three sides. This will align the ring stack.

18. While holding the Alignment Fixture in contact with the rings tighten each screw until they are snug. Avoid tightening one of the screws all of the way down before tightening the other two screws. Over tightening one screw will cause the stack to go out of alignment.

19. Continue tightening the screws sequentially until they are tight. It is not necessary to exert excessive force on the screws but they need to be tight enough to keep the stack from moving. If a torque screwdriver is available a final tightening to 12 in/oz is recommended.

Mount the trap assembly onto the RF board

1. Use the following image to orient the trap on the RF board.

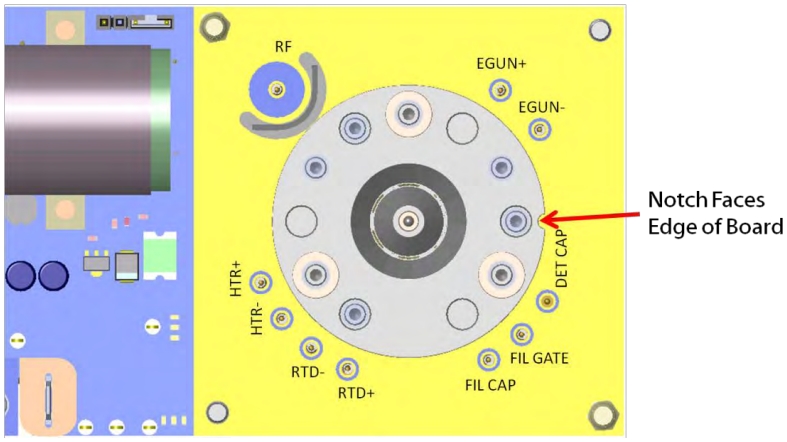


Figure 8-19 Trap orientation on RF board

2. Position the trap assembly so that the notches in the electrodes face away from the RF coil and toward the edge of the board.

3. Install the trap mounting screws. Tighten them snuggly but do not over tighten the screws.

Trap final reassembly

1. Install the EGUN mount. Use the following image to orient the EGUN mount on the trap.

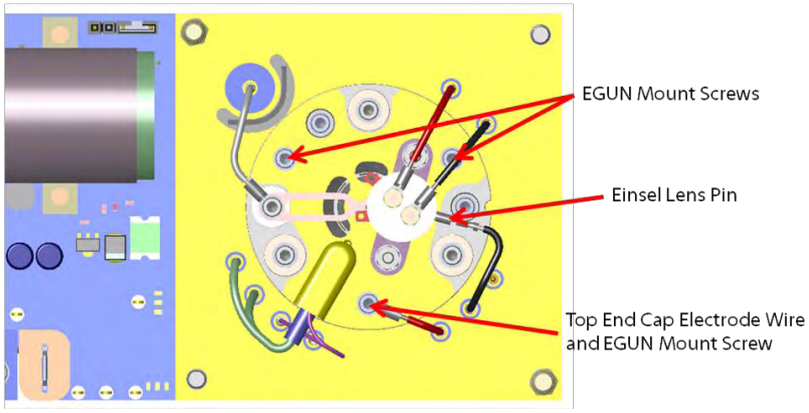


Figure 8-20 EGUN mount orientation

2. One of the screws on the EGUN mount is also used to hold the Top End Cap Electrode Wire.

3. Install the other two screws first then install the screw with the Top End Cap Electrode Wire. Slide the Top End Cap Electrode Wire onto the connector on the RF board.

4. Slide the Red and Black Filament wires onto the connectors on the RF board. Install the black wire onto the FIL- pin and the red wire onto the FIL+ pin.

5. Use the 1/8" hex nut driver to make sure the nuts on top of the filament are still tight.

6. Slide the RTD wires onto the pins on the RF board.

7. Connect the white RTD wire onto the RTD+ pin and the black RTD wire onto the RTD- pin.

8. Connect the heater wires to the heater connections on the RF board. The labels show HTR+ and HTR-. These labels are for convenience in trouble shooting. There is no plus or minus orientation for the heater. Connect one of the heater wires to the HTR+ and the other to HTR-.

9. Install the RF wire, screw, polyimide spacer and RF tab. The tab must be positioned so it is in contact with the top pin of the Center Electrode (football).

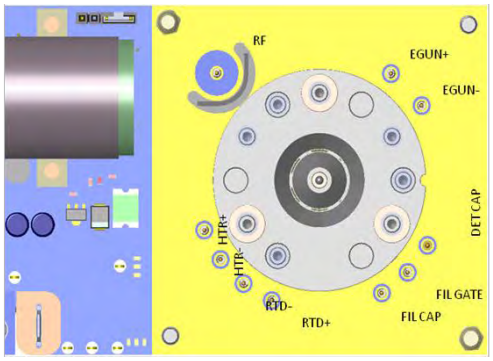
10. Slide the RF wire onto the pin on the RF board.

11. Slide the Einsel Lens wire onto the pin on the Einsel Lens and onto the connector on the RF board.

Filament replacement

1. Follow the instructions in the Remove ion trap/RF module section of this chapter to remove the ion trap from the vacuum chamber.

2. Slide the Red and Black Filament wires off the pins on the RF board. The following image shows the position of the electrical connections on the RF board.



RF	RF Wire
EGUN+	Filament Red Wire
EGUN-	Filament Black Wire
DET CAP	No Connection
FIL GATE	Einsel Lens Wire
FIL CAP	Top End Cap Electrode Wire
RTD+	Black RTD Wire
RTD-	White RTD Wire
HTR-	Either Heater Wire
HTR+	Either Heater Wire

Figure 8-21 Trap wire connections

3. Squeeze the tabs on the filament clip with needle nose pliers and slide the filament straight up and out of the EGUN barrel.

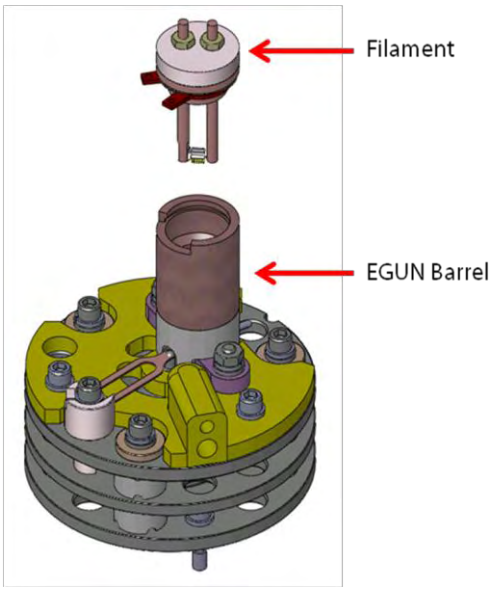


Figure 8-22 Filament removal

4. Slide the new filament assembly into the EGUN barrel. Squeeze the filament clip with needle nose pliers and gently press the filament down until it snaps into place. A correctly installed filament will sit level and with slight sideways pressure it will be able to rotate.

5. Use the 1/8" hex nut driver to install the red and black wires onto the top of the filament (if they did not come pre-installed on the new filament). Ensure that the red wire aligns with the Egun + pin on the RF board and on the brown plastic part of the filament assembly. Make sure the black wire aligns with the Egun – pin on the RF board and on the brown plastic part of the filament assembly.

6. Use the 1/8" hex nut driver to make sure the nuts on top of the filament are tight.

7. Slide the wires of the new filament onto the pins on the RF board.

Einsel lens maintenance

Einsel lens cleaning procedure

1. Follow the instructions in the Remove ion trap/RF module section of this chapter.

2. The following image shows an exploded view of the einsel lens assembly.

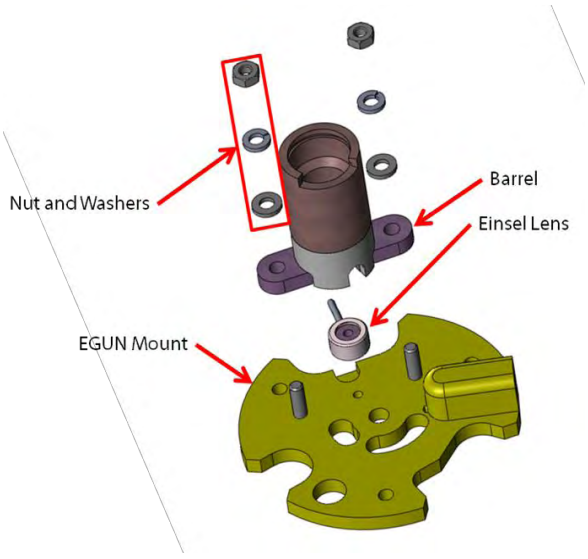


Figure 8-23 Einsel lens exploded view

3. Follow the instructions in the Filament Replacement section and remove the filament assembly.
4. Slide the Einsel Lens wire off the Einsel Lens and off the pin on the RF board. Set the wire aside on a clean lint free surface.
5. Use the provided 5/32" hex nut driver to remove the Einsel Lens nuts.
6. Lift the barrel off.
7. The Einsel Lens is comprised of a brazed together ceramic spacer and a stainless steel lollipop shaped electrode. Remove the Einsel Lens from the Barrel.
8. Clean the Barrel and the Einsel Lens using soap (Alconox works well), water and a soft bristle brush or cotton tipped swab.
9. Thoroughly rinse the parts with deionized water and allow them to dry.

Einsel lens assembly

1. Place the Einsel lens assembly into the Barrel with the side showing more metal down and the stem passing through the slot in the Barrel.
2. Position the Barrel with the installed Einsel Lens parts over the threaded studs on the EGUN Mount. The stem should point away from the center of the trap and toward the closest edge of the board.
3. Install the two nuts using the 5/32" hex nut driver. Tighten them so the Barrel is secure. Do not over tighten the nuts as this may damage the Einsel Lens, Barrel or EGUN Mount.

Electron multiplier detector replacement

Remove the electron multiplier detector

1. The type of electronic detector used in the TRIDION is a continuous dynode electron multiplier detector. It will be referred to as the detector in this section of the manual.

2. Follow the instructions in the Remove ion trap/RF module section of this chapter.

3. The following image shows an exploded view of the ion trap/RF module from the perspective of the outside of the vacuum end cap. Use this image as a reference for component identification while replacing the detector.

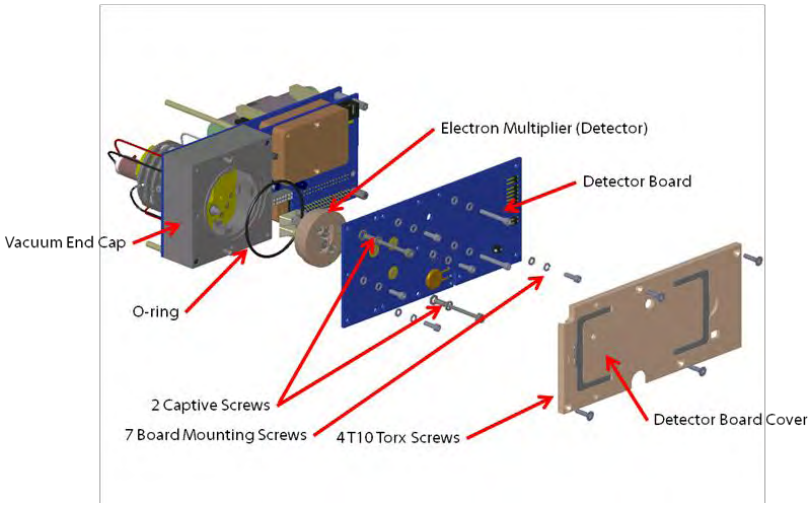


Figure 8-24 Electron multiplier replacement diagram

4. The electron multiplier is located under the white Detector Board Cover and under the Detector Board.

5. Use the T10 Torx driver to remove the four flat head screws that hold on the white Detector Board Cover. The cover should come off with the screws. Set the cover aside.

6. Remove the captive screws that were loosened during the ion trap/RF module removal from the TRIDION.

7. Use the 5/64" hex driver to remove the screws that hold the Detector Board to the ion trap/RF module.

8. Use the 3/32" hex driver to remove the remaining screws that hold the Detector Board to the ion trap/RF module.

9. Carefully pull the Detector Board off the ion trap/RF module. Some of the connectors are tight and can be difficult to pull out. If the board is twisted or slid sideways the glass of the detector can come in contact with the metal part of the vacuum end cap and can break. If this happens the detector cannot be used.

10. Be careful to not damage the O-ring.

11. The O-ring and the area inside of the O-ring are in the vacuum chamber. Any user that will be handling any parts internal to the vacuum chamber needs to be wearing lint free laboratory gloves.

12. Use the 3/32" hex driver to remove the screws that hold the Detector to the Detector Board.

Reassemble the electron multiplier detector

1. Position the new detector and using the screws in the detector mounting holes secure the new detector to the detector board.

2. The following image shows a detector side view of the detector board.

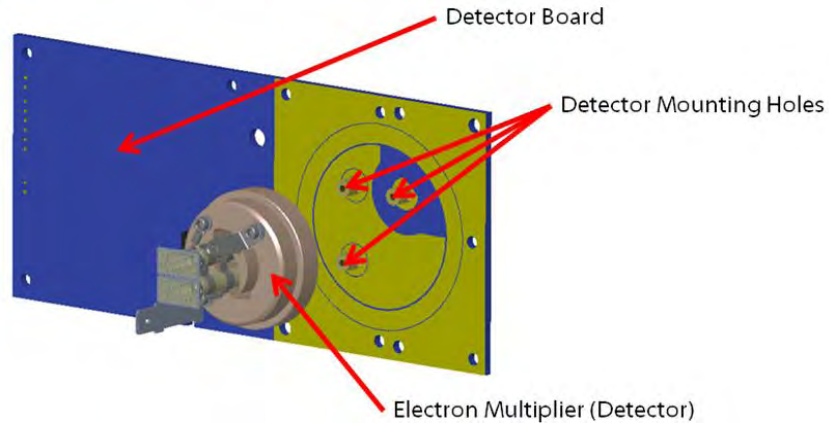


Figure 8-25 Electron multiplier detector mount to detector board

3. Insert the detector into the vacuum chamber and simultaneously plug the electrical connections of the detector board into the ion trap/RF module.

4. Using 3/32" driver replace the smaller screws.

5. Reinstall the captive screws that hold the ion trap/RF module in the TRIDION.

6. Reinstall the 7/64" driver replace the larger screws.

7. Position the white Detector Board Cover and using the T10 Torx driver reinstall the flat head screws.

Install the ion trap/RF module

1. Insert the trap assembly into the vacuum chamber, ensuring that the alignment pins slide into the holes on the vacuum chamber and that the vacuum chamber O-ring stays in place.

2. Using a 7/64" hex driver screw the captive screws into the vacuum chamber end cap.

3. Place the front cover of the TRIDION in place by positioning the bottom edge and pushing the top edge into place. Use the 7/64" hex driver to install the five screws along the bottom edge of the cover.

GC injection port maintenance

1. The following sections provide instructions on maintenance of the GC injection port.

2. The following image shows an exploded view of the GC injection port. Refer to this image while doing maintenance on the GC injection port.

Figure 8-26 Exploded view GC injection port assembly

Accessing the GC injection port

1. The following steps are required before doing any maintenance on the GC injection port.
2. Unscrew the plastic cover from the Universal Interface.
3. Using the Ring Removal tool remove the stainless steel Interfacing Mounting Ring Nut.
4. Pull the Universal Interface out of the top of the TRIDION.
5. After removal of the Universal Interface the GC injection port is accessible.

Septum replacement

1. Make sure the instrument is cool.
2. Remove the Septum Nut from the top of the GC injection port by unscrewing the nut.
3. Remove the old Septum.
4. Install the new Septum.
5. Replace the Septum Nut. Make sure the nut is tight.

Injection liner and seal cleaning or replacement

1. The injection port must be warm to replace the Injection Liner and/or Seal.
2. Before heating the injection port remove the Septum Nut.

3. It is preferable to load a custom method that heats only the Injection Port. The method should have all of the other temperatures set to off and the Injection Port set to 50°C. Allow the temperature to reach 50°C.

4. After the Injection Port has reached 50°C grasp the Injection Liner and pull it out of the Injection Port.

5. Remove the Liner Seal from the bottom of the Liner.

6. Replace the Liner and Seal with the new Liner and/or Seal.

7. Remove the Septum from the old Liner and insert it into the new Liner.

8. There are two separate Liners that can be used in the TRIDION. There is a liner for SPME type injections and a larger volume liner for small liquid injections.

9. Reinstall the Septum Nut. Make sure the Septum Nut is tight.

10. The Liner has a deactivated surface. It can be cleaned with normal solvents like methanol or hexane. Use of aggressive acid or base will damage the liner coating and result in poor performance for active chemical compounds. If the Liner appears to be scratched or damaged in any way it is recommended that the Liner be replaced.

11. Re-install the Universal Interface by positioning it with the flat side of the port lining up with the flat side of the opening. Make sure the assembly is plugged into the board. Reinstall the stainless steel Interface Mounting Ring Nut and the protective cover.

Chapter 10

9 Troubleshooting

This chapter describes basic troubleshooting of the TRIDION.

TRIDION will not turn on

1. Press the power button firmly for ten seconds (see figure 5.1).
2. Check the batteries for proper installation. Remove and re-install the batteries or replace them with new/charged batteries.
3. Check the external power source for proper function and verify that the voltage regulator meets the correct specifications (see the section called *Power Supply and Battery*). Remove the power source connector from the TRIDION and re-insert it snuggly.

TRIDION will not turn off

1. Press the power button firmly for ten seconds (see figure 5.1).
2. Re-set the on-board computer (see the section called Re-set the on-board computer in the Advanced Operations chapter of this manual)

TRIDION cannot maintain vacuum

1. If recent maintenance was performed on the instrument where the vacuum chamber was opened, ensure that the O-ring seal to the vacuum chamber is properly seated to maintain a proper seal.
2. Refer to the Instrument Operation chapter under the Advanced/Status/Diagnostics/Mass Spectrometer section for images of the screens.
3. The turbo pump information is shown on the Mass Spectrometer tab.
4. Verify that the frequency of the Turbo Pump is not increasing (see Hz column to the right of Turbo Pump, it should progress until 1500 +/- 10 Hz). If the frequency is increasing, wait to see if the vacuum can be established. If the frequency is not increasing or the vacuum is not established, continue with the next step.
5. Restart the instrument. Another attempt may be successful. If the vacuum is not achieved after the second try, contact TORION Technologies.

GC baseline is noisy, or drifts upward

1. A noisy chromatogram suggests chemical contamination. Contamination can arise from dirty components such as from the SPME fiber, injector port, chromatographic column, vacuum chamber, or ion trap.

2. The following list provides possible solutions for correcting a noisy GC baseline.

    a. Clean the SPME fiber (see the section Prepare the CUSTODION SPME syringe for sampling).
    b. Replace the SPME fiber.
    c. Clean the ion trap and electron gun (see the section called *Trap maintenance procedures*).
    d. Bake out the injector and column (see the section called *Bake out the GC injection port and* column). If the problem persists, the injection port liner, the septum, or the column may need to be replaced. To replace any of these components contact TORION.
    e. Bake out the vacuum chamber, contact TORION.

GC peaks are asymmetric

1. Please note: chromatographic peaks during a PERFORMANCE VALIDATION run will look asymmetric and will most likely have peak tailing. This is not indicating a problem.

2. Chromatographic peaks should be symmetric and Gaussian. Asymmetric and non-Gaussian peaks typically result from an overloaded column, a degraded column, an incompatible solute/column combination, or incorrect instrument parameters or operation.

3. Improving peak shape is important for the best confidence in identifying target chemicals; however, asymmetric peaks will not necessarily prevent identification. Some compounds are generally detected as asymmetric peaks, in which case the chemical agent library can be calibrated to compensate.

4. Asymmetric peaks may indicate problems with sampling, delivery, separation, or ionization. Fronting and tailing are useful indications of possible causes.

Observation	Example	Possible cause
Fronting		The sample is too concentrated and is saturating the column, allowing some of the sample to elute faster than expected.

5. The following list provides possible solutions to correct for fronting.

    a. Use a faster injection time by leaving the SPME fiber extended for a much shorter time during the introduction of the sample. To do this, extend the SPME fiber when prompted by the screen and then immediately retract the fiber and remove the syringe without waiting for the additional prompts.

b. Collect the sample using the headspace method described in the section called Using the CUSTODION for obtaining a sample for analysis.
c. Dilute the sample.
d. Use a sample solvent with less affinity for the SPME fiber. For example, replace acetone with water if possible.

Observation	Example	Possible cause
Tailing		(1) A surface to which the sample is exposed is adsorptive. This can arise because the injector, column or transfer lines are not deactivated well enough, or these surfaces become contaminated with nonvolatile components in the sample. (2) Dead volume or cold spot in the injection port.

6. The following list provides possible solutions to correct for tailing.

    a. Try baking out the injector and column (see the section entitled Bake out the GC injection port and column).
    b. Clean the injection port liner with appropriate solvents (see the section entitled GC injection port maintenance).
    c. Replace the injection port liner with a newly deactivated one (see the section entitled GC injection port maintenance).
    d. Replace the column, contact TORION.
    e. Increase the split flow rate.

7. A peak may be non-Gaussian if too few data points are obtained. Too few points result from low sample concentration, low ionization yield, incorrect detector voltage, detector malfunction, steep temperature gradient in the temperature program, or rapid carrier gas flow rate.

8. The following list provides additional solutions for correcting peak shape due to low concentration.

    a. Analyze a more concentrated sample.
    b. Increase the filament current (increase number of electrons and therefore number of ions, however, the filament may burn out faster).
    c. Increase the detector voltage. This may help slightly, but the noise increases as well. Too high of a detector voltage can permanently damage the instrument and will age the detector faster.
    d. Replace the detector with a new one.
    e. Reduce the temperature programming rate to broaden the bands in the column and thereby broaden the peaks.
    f. Reduce the carrier gas flow rate to broaden the bands in the column and thereby broaden the peaks.

GC peaks are eluting late

1. When users notice that the GC peaks are eluting late or early this indicates a change in air flow or pressure. A change in air flow or pressure can be due to several things. If the peaks are eluting **late** the following is a list of things for users to verify:
   a. Verify the helium source still has an adequate amount of helium. If using the on-board carrier gas cartridge check the He High Pressure of the system which will indicate if the cartridge is empty. To do this:

      i Access the Advanced screen (see the Advanced Operations chapter for instructions).

      ii Select the **Status/Diagnostics** screen.

      iii Select the Gas Chromatography tab and the following screen will be displayed.

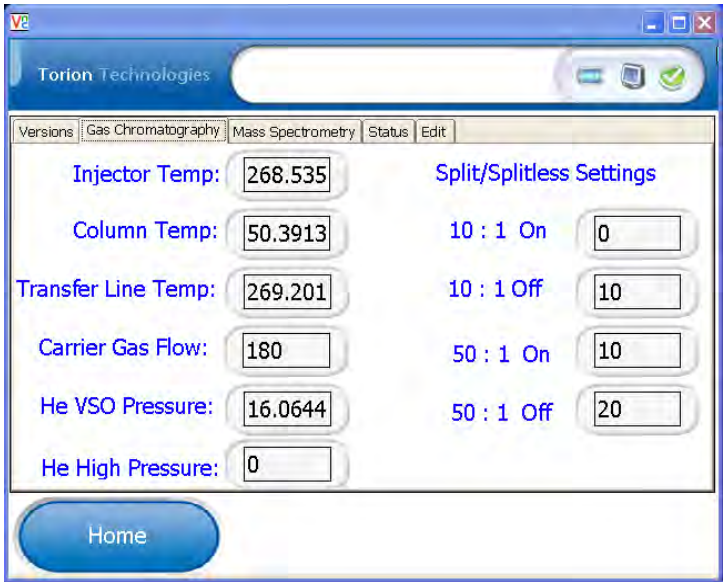


Figure 10-1 Gas Chromatography tab

      iv Check the He High Pressure read back. When the helium cartridge is full this reads approximately 2500 and 0 when it is empty. If the cartridge is empty replace it with a new one (see Change the carrier gas cartridge in the Other Operations chapter).

   b. If using an external helium source verify that the source still has an adequate amount of helium and that the pressure regulator is set to 80 psi. Also verify that none of the carrier lines and/or connections are leaking.

   c. Verify that the Merlin septum is not leaking. If it is leaking replace it with a new one, see section Septum Replacement in the Service chapter.

Acquired mass spectra are noisy

1. If the mass spectra are noisy, the chromatogram will probably be noisy as well. A noisy mass spectrum may result from some of the problems discussed in the section called GC baseline is noisy or drifts upwards or may be caused by the problems discussed in this section.

2. Mass spectral noise may be the result of poor noise filtering or chemical contamination that convolutes the spectra.

3. Noisy spectra can result from an incorrect detector voltage, higher detector voltage increases sensitivity, it also increases random noise. The electron gun current may also be too high, producing too many ions for the trap (see the section called Recommended Operating Parameters).

4. Noisy spectra can result from an old or faulty detector (see the section called Electron multiplier detector replacement).

5. Noisy spectra can result from a dirty ion trap (see the section called Trap maintenance procedures on removing and cleaning the trap).

6. Noisy spectra can result from impure carrier gas. Replace the gas cartridge with a new cartridge or external gas line and follow the instructions in Bake out the GC injection port and column.

Note

Noisy spectra may be improved with the noise filters included as instrument parameters.

Results are not reproducible

1. Results may be irreproducible when the operating parameters are outside the suggested ranges (see the section called Recommended Operating Parameters) or when the components are dirty or faulty. Some suspected parameters include: detector voltage, electron gun current, column and injector settings. The suspected components may include the column, injector port, ion trap, or the SPME syringe or fiber. The sampling technique is also critical for reproducibility. The following list provides possible solutions for correcting irreproducibility.

    a. Re-extract and analyze the sample with a new SPME fiber or after cleaning the SPME fiber (see the section called Prepare the CUSTODION SPME syringe for sampling).
    b. Allow the instrument to warm-up for several minutes before analyzing a set of samples.

    c. Run a standard and verify that the mass spectrometer and chemical library calibrations are still good; make adjustments as necessary, and re-filter the irreproducible data with the new calibrations.

    d. Evaluate the extraction procedure and eliminate any variations such as inconsistent extraction time, temperature, or agitation procedure.

There is no instrument signal

1. Lack of signal is typically observed when the electron gun filament burns out or when the detector malfunctions or needs replacement. The signal will either be absent or appear as a baseline. When this happens the instrument may be sent to Torion Technologies, or the user may replace the filament or detector by following the instructions in the Service chapter.

Acquired mass spectra are not correct

There are a few different things that may cause the acquired mass spectra to be incorrect. For troubleshooting follow the steps below:

1. Perform 3 analytical runs using the CALION Standard Mix. Analyze the 3 runs to determine if the acquired masses (although incorrect) are the same for each run (± 1 amu). If from run to run the masses are shifting dramatically contact Torion Technologies. If the masses (although incorrect) are staying the same (± 1 amu) from run to run continue to perform the steps below until the problem is corrected.

2. When the acquired mass spectra are not correct the TRIDION should be recalibrated (see section Performance Validation Button in the Instrument Operation chapter). After performing the Performance Validation run the CALION mix again as a sample to verify that the acquired masses are now correct. If needed repeat the Performance Validation a couple times.

3. Another problem that can contribute to incorrect mass assignments is a dirty trap. For trap removal and cleaning instructions see the Service chapter. After cleaning the trap perform a Performance Validation, then analyze the CALION Mix using the TRIDION and ensure that the acquired mass spectra are correct.

4. If none of these steps corrected the acquired mass spectra contact Torion Technologies.

SPME fiber came off inside the GC inlet

1. Occasionally a SPME fiber can come off inside the GC inlet. This can happen when the fiber is getting old, if the fiber is used in an incompatible solvent it swells or breaks, if the SPME syringe is pulled out of the inlet while the fiber is exposed etc.

2. It is very important that the SPME fiber is removed from the inlet immediately. If the fiber is left inside the inlet subsequent fibers that are inserted in the inlet might break off because there is not enough room for the fiber. Fibers left inside the inlet can also allow fiber debris to block the GC or even damage the GC column.

3. To remove a SPME fiber from the GC inlet follow the steps in the GC injection port maintenance section of the Service chapter. Ensure that the entire fiber is removed from the inlet, Merlin Septum and GC liner.

TRIDION fails Performance Validation

See the section Correcting failed auto calibration (Performance Validation) in the Advanced Operations chapter.

TRIDION fails to identify a compound

It is possible that the TRIDION can fail to identify a compound that is actually present (a false negative identification). There are several reasons why the TRIDION would fail to identify the compound. Address each of the possibilities listed below:

1. The target compound did not elute within the correct retention time window. This may happen if:

    a. The retention time window set in the library may be too small.

    b. The TRIDION may be running out of helium.

2. The target compound does not have the correct mass spectrum. If this is the case see the troubleshooting section 'Acquired mass spectra are not correct' to solve this problem.

TRIDION falsely identified a compound

It is possible that the G-7 can identify a compound that is actually not present (a false positive identification). There are a couple reasons why this may happen.

1. The mass spectrum of the false positive compound might match the mass spectrum of a compound that is actually present. If this is the case, see if there are additional unique ions that can be added to the library for more selective identification.

2. The mass spectrum of the false positive might be present in the background noise. This will happen especially when running compounds in a complex matrix such as gasoline or diesel.

TRIDION fails to reach set temperatures

If at anytime the TRIDION fails to reach temperatures set in the GC settings contact Torion Technologies.

TRIDION is unable to run on battery power

If the TRIDION has previously been successful at running on battery power ensure that the batteries have been fully recharged and are making proper connection with the TRIDION. Also ensure that the batteries being used still have enough power left to run the TRIDION. If the instrument is still unable to run on battery power contact Torion Technologies.

TRIDION suddenly powers down

If the TRIDION was running on battery power, the life of the battery has been exceeded. Replace the batteries, or switch to alternative power and perform a blank run on the TRIDION before continuing with analysis. If the TRIDION was running on alternative power ensure that the power is properly connected. Once the power is properly connected perform a blank run on the TRIDION before continuing with analysis.

TRIDION is dropping data points

Under typical parameter settings the TRIDION should produce ~7 – 10 scans per second. If the TRIDION is dropping data points contact Torion Technologies.

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